ANNUAL REPORT

2001

MTA SZFKI

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS

of the Hungarian Academy of Sciences, Budapest, Hungary

ANNUAL REPORT

2001

Host institute of the KFKI Condensed Matter Research Centre

CENTRE OF EXCELLENCE

MTA SZFKI

RESEARCH INSTITUTE FOR SOLID STATE PHYSICS AND OPTICS

of the Hungarian Academy of Sciences, Budapest, Hungary

Research Institute for Solid State Physics and Optics
of the Hungarian Academy of Sciences

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ANNUAL REPORT 2001

Edited by **L. Csillag, E. Kántor, G. Konczos, B. Selmeci, I. Tüttő,**

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Dear Reader,

It is my pleasure to hand over the Annual Report of the Research Institute for Solid State Physics and Optics in 2001.

Our institute was founded by the Hungarian Academy of Sciences in 1981 as part of the Central Research Institute for Physics. In 1992 we became an independent institute and along with our status changed our name as well: "Research Institute for Solid State Physics". In 1998 the Crystal Physics Laboratory of the Hungarian Academy of Sciences joined our institute as a part of the reorganisation process of the academic institutes and at the same time our name has been altered to "Research Institute for Solid State Physics and Optics". The main profile of the institute is basic research in the fields of theoretical and experimental solid state physics and materials science including metal physics and liquid crystal research, theoretical and experimental optics including laser physics and the interaction of light with matter. Our experimental research activity is connected to unique methodologies like X-ray diffraction, NMR-, Mössbauer-, and optical spectroscopy and neutron scattering experiments at the KFKI Research Reactor. Some of our research (R & D) activities are more closely related to applications, first of all in the fields of optical thin films, laser applications, crystal growing technologies and metallurgy.

Our research activity is financed by the Hungarian Academy of Sciences and by national and international research funds like the Hungarian National Research Fund (OTKA) and also through individual projects. Since Hungary has joined the EU 5th Framework Programme, the international co-operation has become even more important for the scientific work of our research groups. Our institute, as the host of the KFKI-Condensed Matter Research Centre (KFKI-CMRC) is taking part in the "*Centre of Excellence*" programme of the European Union. We are in active contact with a great number of research institutions and universities. More than half of our publications feature foreign co-authors, indicating the significant role of these collaborations. The different EU, ESF, COST, NATO and other international projects play an ever increasing role in our research activity. The share of these international resources in our budget shows a rapid increase compared to previous years (EU funds in 2000 were 8%; in 2001 13% of our budget). A remarkable increase can be observed concerning investments, which is very appealing taking into account the average age of our equipment. We are participating in two projects of the National Research and Development Program (NKFP); one is concerning nanotechnology, while the other is concentrating on the study of environmental pollution caused by atmospheric aerosols.

Our institute has a long tradition in graduate and to a larger extent in post-graduate education. Details of this activity are also given in this Annual Report. We have published about 180 papers in high quality international journals and conference proceedings. The number of publications is similar to that of the previous years. In 2001 three of our scientists

have become Doctors of the Hungarian Academy of Sciences (DSc) and two of our colleagues have been elected to the members of the Hungarian Academy of Sciences.

I hope that this booklet gives useful information to the reader. The key figures help you to get a general overview of our institute as a whole. The Annual Report contains the e-mail addresses of our scientists as well, to make it easier to get in contact with them directly. For further information please visit our WEB page at www.szfki.hu.

Budapest, December 1, 2001

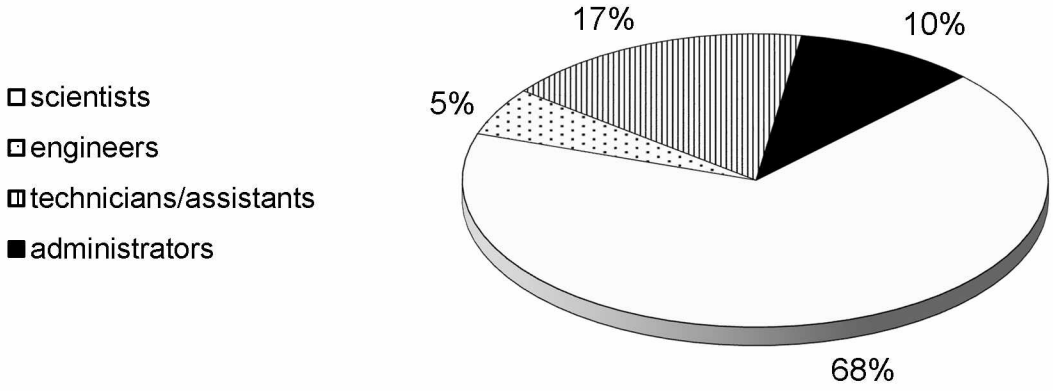
János Kollár

Director

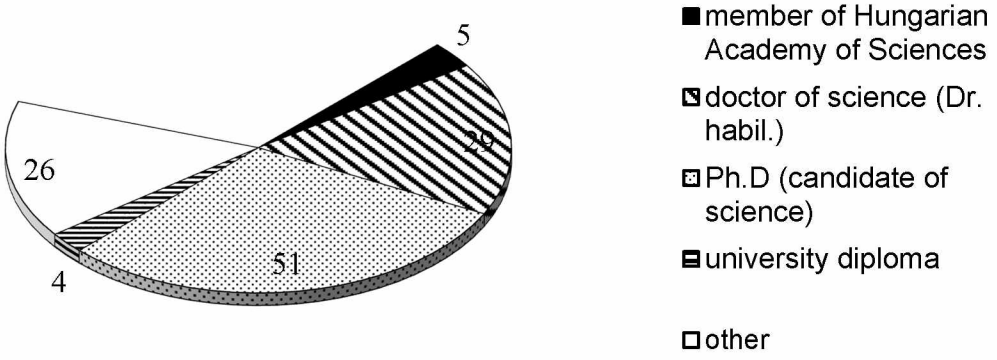
Key figures

Permanent staff of the Institute: 170 employees. Its distribution:

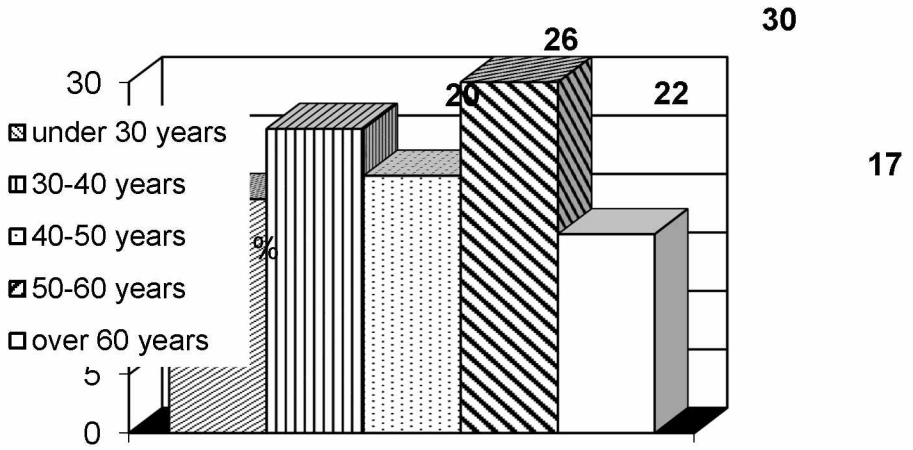
a) by professions:



b) by scientific titles/degrees:

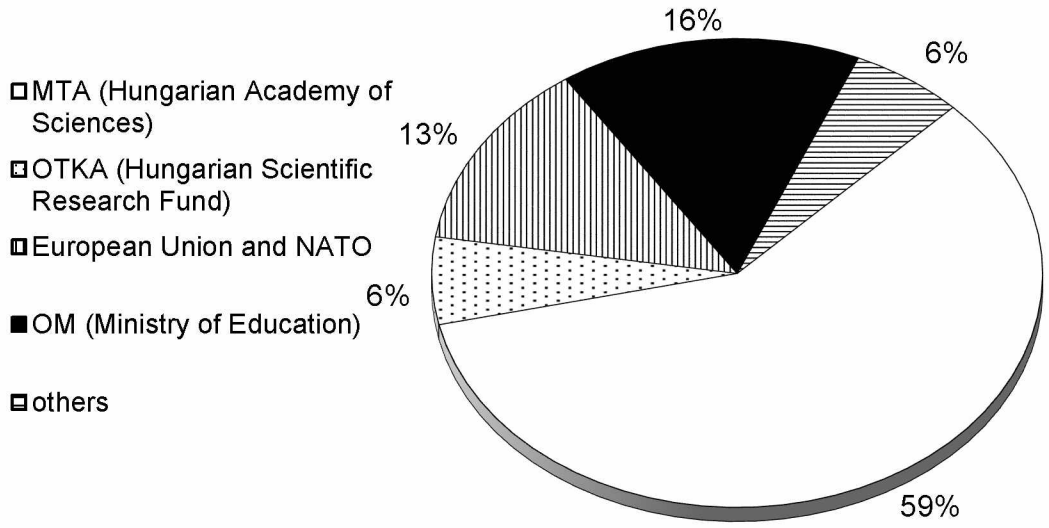


c) by ages:

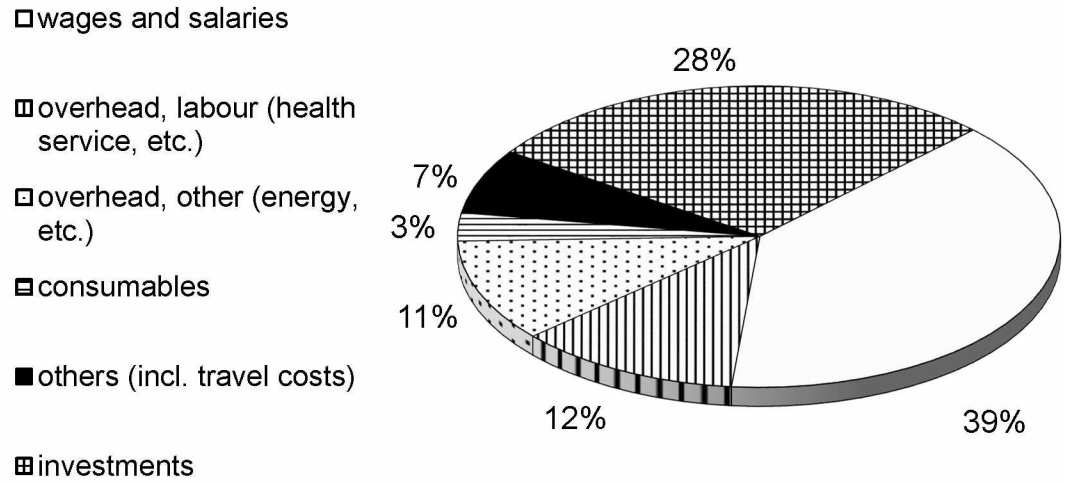


Financial management

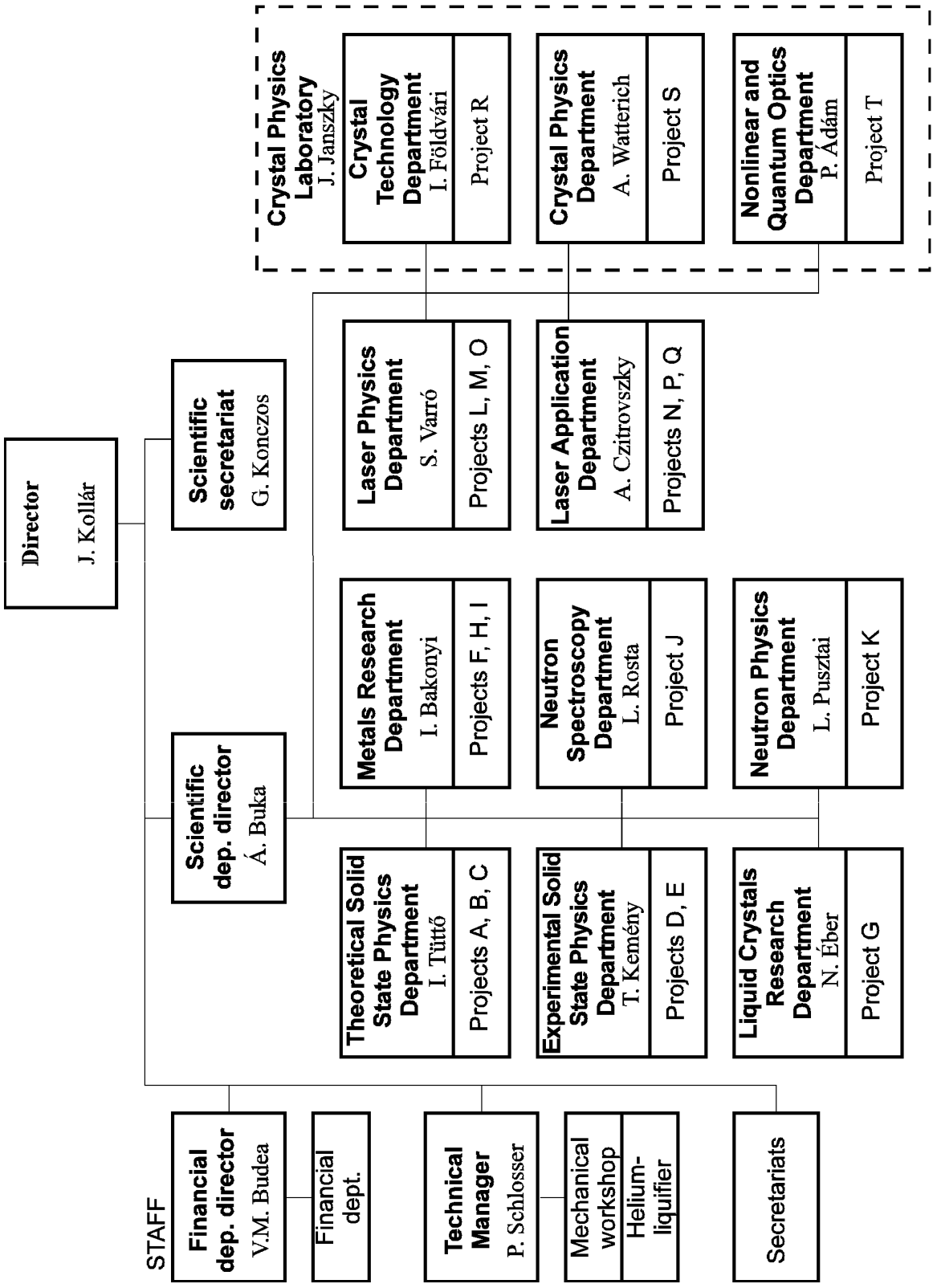
a) Sources of operation costs:



b) Distribution of expenditures:



Structure of the Research Institute for Solid State Physics and Optics



A. STRONGLY CORRELATED SYSTEMS

J. Sólyom, G. Fáth, Ö. Legeza, K. Penc, A. Rákos, K. Vladár, F. Woynarovich, A. Zawadowski[+]

Low dimensional magnetic models. — We continued studying the low-energy excitations (with an effective size of the order of the chain length) in the isotropic Heisenberg chain. In this case the Bethe Ansatz equations loose their usual structure because of the incompleteness of the scattering procedures. We have determined the structure of such excitations with different types of symmetries (triplet and singlet).

Antiferromagnetic Heisenberg spin chains in a sufficiently strong magnetic field are Luttinger liquids, whose parameters depend on the actual magnetization of the chain. We calculated precise numerical estimates of the Luttinger liquid parameters by determining the critical exponents of the correlation functions in magnetization profiles for S=1/2, 1, 3/2 chains using the density matrix renormalization group method. For S=1/2 the numerical results show excellent agreement with exponents calculated from conformal invariance and Bethe Ansatz.

We have studied models of spin ladders composed of S=1/2 spins coupled along the rungs, diagonally, and by plaquette interactions. We argued that in case of a ladder one can define two kinds of Haldane states. Both of them possess some kind of topological long-range order, but the two sectors differ in topological quantum numbers, and hence in order parameters. The two topological sectors are necessarily separated by a phase transition. The transitions was analyzed numerically using the density-matrix renormalization group algorithm, computing the topological (string) order parameters in the ground state.

Fermionic and bosonic models. — We have developed a new code for the momentum space version of the density-matrix renormalization group (DMRG) algorithm in order to increase the efficiency of the method. It was applied to the one-dimensional Hubbard chain as well as various molecules (CH_2, H_2O, NaF, LiF) and studied their corresponding one-dimensional lattice models up to 40 sites. Since this new method is still in a development stage we have carried out most of our test calculations on molecules in the framewok of an international scientific cooperations. Several new ideas and modifications were introduced into the algorithm, which allowed us to reduce significantly the computational time and the computer memory requirement. We have also analyzed the convergence of the new approach when second excited states are calculated for systems with singlet or triplet ground states. Through the cooperation of our KFKI-CMRC project we have worked out basic changes in the algebra of DMRG in order to study the four-component relativistic Dirac-Fock equations. We have also applied DMRG for the one dimensional Hubbard model for short chain lengths. Detailed investigation of such models with the algorithm is in progress. Based on the models studied so far we can conclude that DMRG seems to provide a more efficient way to treat long range electron interaction and it could become the most widely applied algorithm in quantum chemistry.

In some insulators the electrons can choose between degenerate orbitals to occupy, and this leads us to models where not only the usual spin, but also the orbital degrees of freedom should be taken care of. While usually these models are highly anisotropic in couplings, it some particular cases we obtain a fully symmetrical model - the simplest one is the SU(4) symmetric "Heisenberg model" of S=1/2 spin with two orbitals to choose from. The physics

[+] Permanent position: Budapest University of Technology and Economics

of the SU(N) Heisenberg lattice models is not well understood. We study the SU(4) model on the triangular lattice with nearest and next nearest exchange couplings with different methods, and find evidence of a quantum phase transition between an ordered 4-sublattice state into a disordered resonating liquid of SU(4) singlet plaquettes as the coupling parameters change.

We studied the thermodynamics of surface states, in Bethe Ansatz solvable systems. As an example we solved the 1D delta Bose gas with an attractive surface-potential, and we have calculated the effect on the free-energy in the interaction of the surface bound particles and the bulk.

Kondo problem. — We have studied the role of the electron-hole symmetry breaking in different kind of Kondo problems. Generally it was assumed that breaking that symmetry the infrared divergencies are not affected. Examining through a couple of cases it is shown that the symmetry breaking in some cases may lead to observable modifications while in other cases not.

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Grants

OTKA[1] T 022607 Completely integrable quantum chains (F. Woynarovich 1997-2001)

OTKA T 030173 Theoretical study of magnetically or electrically low-dimensional models (J. Sólyom, 1999-2002)

OTKA F031949 Effect of magnetic field on the behavior of quantum spin chains (G. Fáth, 2000-2003)

OTKA F 032231 Study of coupled spin and fermion chains with the density matrix renormalization method (Ö. Legeza, 2000-2003)

OTKA D32689 (postdoctoral). Spin and orbital ordering in frustrated vanadium oxydes and sulphides (K. Penc, 2001-2002)

Publications

Articles

A.1. E. H. Kim*, G Fáth, J. Sólyom, and D. J. Scalapino*: Phase transition between topologically distinct gapped phases in isotropic spin ladders. *Phys. Rev.* **B62**, 14965-14974 (2000).

[1] OTKA=Hungarian Scientific Research Fund

* The author is not a member of the Research Institute for Solid State Physics and Optics staff

A.2. F. Mila*, K. Penc: Model calculations for 1D correlated systems. *J. Electron Spectrosc.* **117**, 451-467 (2001).

A.3. G. Fáth, Ö. Legeza, and J. Sólyom: String order in spin liquid phases of spin ladders. *Phys. Rev. B* **63**, 134403/1-5 (2001).

A.4. O. Újsághy*, K. Vladár, G. Zaránd* and A. Zawadowski: The Role Of Electron-Hole Symmetry Breaking in the Kondo Problems, J. Low-Temp. Phys., accepted for publication

Conference proceedings

A.5. J. Sólyom: Phase diagram of spin ladder models and the topology of short valence bonds. In: *Proc. NATO ARW BLED 2000 Open Problems in Strongly Correlated Electron Systems,* Kluwer Academic Publisher, 2001, pp. 91-100

A.6. K. Penc, W. Stephan*: Spin-charge separation in the Sr_2CuO_3 and $SrCuO_2$ chain materials. In: *Proc. NATO ARW BLED 2000 Open Problems in Strongly Correlated Electron Systems*, Kluwer Academic Publisher, 2001, pp. 303-309

A.7. P. Fazekas, H. Berger*, L. Forró*, R. Gaál*, I. Kézsmárki*, G. Mihály*, M. Miljak*, K. Penc, F. Zámborszky*: Non-magnetic Mott insulating phase and anomalous conducting state in barium vanadium trisulphide. In: *Proc. NATO ARW BLED 2000 Open Problems in Strongly Correlated Electron Systems*, Kluwer Academic Publisher, 2001, p. 387-392

A.8. J. Sólyom: Luttinger liquid behaviour of nanotubes. In: *Proceedings of the School and 2nd Workshop on Nanotubes & Nanostructures 2000, Atti di Conferenze*, Vol. 74, Italian Physical Society, Bologna, 2001, pp. 85-102

See also C.18.

B. COMPLEX SYSTEMS

F. Iglói, R. Juhász[#], N. Menyhárd, A. Sütő, P. Szépfalusy

The principal interest of this group is the theoretical investigation of different aspects of equilibrium and non-equilibrium statistical physics and quantum systems.

Phase transitions and critical behaviour. — We have used a strong disorder renormalization group (RG) scheme to study singular quantities in the Griffiths phase of random quantum spin chains. For the random transverse-field Ising spin chain we have extended Fisher's analytical solution to the off-critical region and calculated the dynamical exponent exactly. Concerning other random chains we argue by scaling considerations that the RG method generally becomes asymptotically exact for large times, both at the critical point and in the whole Griffiths phase. This statement is checked via numerical calculations on the random Heisenberg and quantum Potts models by the density matrix renormalization group method.

We have studied the critical behavior of the q-state Potts model with random ferromagnetic couplings. Working with the random cluster representation the partition sum of the model in the large-q limit is dominated by a single graph, the fractal properties of which are related to the thermodynamical singularities of the random Potts model. This optimization problem, connected with the search of the dominant graph, is studied on the square lattice by simulated annealing and by a combinatorial algorithm. Critical exponents of the magnetization and the correlation length are estimated and conformal predictions are confronted with numerical calculations. We have investigated nonequilibrium kinetic Ising models in a *locally* spin-anisotropic environment. The mostly numerical results indicate a drastic change in the phase diagram and critical behavior due to spin anisotropy in one dimension.

Quantum systems. — We showed that in $d > 1$ dimensions the N-particle kinetic energy operator with periodic boundary conditions has symmetric eigenfunctions which vanish at particle encounters, and give a full description of these functions. In two and three dimensions they represent common eigenstates of bosonic Hamiltonians with any kind of contact interactions, and illustrate a partial multi-dimensional Bethe Ansatz or a quantum-KAM theorem. The lattice analogs of these functions exist for $N < L$ where L is the linear size of the box, and are common eigenstates of Bose-Hubbard Hamiltonians and spin-1/2 XXZ Heisenberg models.

We have continued studying the elementary excitations of Bose gases in magnetic and optical traps. A self-consistent model has been worked out which satisfies exact requirements (Ward-identities, Kohn-theorem, compressibility sum rule). We have shown that two excitation branches exist in the model and determined their properties. We have derived a new expression for the entropy production in irreversible processes.

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Grants and international cooperations

OTKA T023791 Nonequilibrium phase transitions (N. Menyhárd, 1997-2001)
OTKA T029552 Study of atomic systems (P. Szépfalusy, 1999-2002)
OTKA T030543 Mathematical study of systems of quantum spins and particles (A. Sütő, 1999-2002)
OTKA T034183 Disordered quantum spin systems (F. Iglói, 2001-2004)
OTKA T034784 Scaling behavior and universality in non-equilibrium systems (N. Menyhárd, 2001-2002)
DAAD-MÖB[2] 200/47 Disordered quantum systems (F. Iglói, 2000-2001)
ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP7: Condensed matter theory (F. Iglói, 2000-2003)

Publications

Articles

B.1. F. Iglói, R. Juhász and P. Lajkó*: Griffiths-McCoy singularities in random quantum spin chains: Exact results through renormalization. *Phys. Rev. Lett.* **86,** 1343-1346 (2001)

B.2. D. Karevski*, Y-C. Lin*, H. Rieger*, N. Kawashima* and F. Iglói: Random quantum magnets with broad disorder distribution. *Eur. Phys. J.* **B20**, 267-276 (2001)

B.3. R. Juhász, H. Rieger* and F. Iglói: The random-bond Potts model in the large-q limit. *Phys. Rev.* **E64**, 056122/1-7 (2001)

B.4. A. Sütő: Nonuniform ground state for the Bose gas. *J. Phys. A: Math. Gen.* **34**, 37-55 (2001), *ibid.* **34**, 6209 (2001)

B.5. J. Reidl*, Gy. Bene*, R. Graham* and P. Szépfalusy: Kohn mode for trapped Bose gases within the dielectric formalism. *Phys. Rev.* **A63,** 043605/1-6 (2001)

B.6. M. Fliesser*, J. Reidl*, P. Szépfalusy and R. Graham*: Conserving and gapless model of the weakly interacting Bose gas. *Phys. Rev.* **A64,** 013609/1-14 (2001)

B.7. J. Hajdu* and P. Szépfalusy : On the production of entropy within the concept of incomplete description of state. *Annalen der Physik* **10,** 429 (2001)

B.8. P. Szépfalusy and G. Szirmai*: The structure of the perturbation series of the spin-1 Bose gas at low temperatures. *Phys. Rev. A,* accepted for publication

[2] DAAD-MÖB = Deutscher Akademischer Austausdienst-Hungarian Scholarship Committee

C. ELECTRONIC STATES IN SOLIDS

J. Kollár, P. Fazekas, K. Itai, A. Kiss[#], I. Tüttő, B. Újfalussy, A. Virosztek[+] , L. Vitos

We have further developed our computational method, the **EMTO-FCD** method (*exact muffin-tin orbitals* combined with the *full charge density technique*) to calculate the electronic structure of bulk solids and surfaces for disordered systems as well. We have used the method to perform calculations for **late transition metal clusters** to show that below a critical size the high surface energy anisotropy stabilizes the icosahedral multiply twinned particle structure against the fcc single crystals. For palladium particles our calculation supports the appearance of ferromagnetic order for non-crystallographic icosahedral symmetry with a small (0.11 μ_B) magnetic moment per atom. Furthermore, we have investigated the elastic property maps of **austenitic stainless steels** and calculated the elastic constants of disordered **Cu-Zn alloys**. Our results are in good agreement with the experimental findings.

As another application of the method, we have studied the relative **stability** of different **perovskite structures**. Within the frame of these studies, the pressure dependent structural properties of $ScAlO_3$ perovskite have been determined. We have found that the $ScAlO_3$ perovskite has orthorhombic structure at 0 K and ambient pressure. This structure is stable relative to the cubic perovskite structure up to pressures of ~ 200 GPa and temperatures of ~ 800 K. We proposed a new parametrization method for perovskite structures; we have shown that this method in combination with *ab initio* total energy calculations is suitable to predict changes in the structural distortion under increasing hydrostatic pressure. Test calculations have been performed for the geophysically important magnesium silicate perovskite.

We have continued the exploration of the phase diagram of the correlated transition metal sulphide $BaVS_3$. Using magnetoresistivity measurements, we determined the pressure dependence of the spin gap up to 15 kbar. The data indicate that the Mott insulating phase of $BaVS_3$ is characterized by spin-orbital resonance. We analyzed the thermodynamic character of the metal-insulator phase transition, and derived a suitable form of the Ehrenfest-Fisher relation, which connects the anomaly of the non-linear magnetic susceptibility with those of the specific heat, and the temperature derivative of the linear susceptibility.

The same kind of thermodynamic reasoning can be applied to f-electron models with coupled orbital and magnetic order parameters, which show a great variety of first-order and higher-order phase transitions, critical lines, and multicritical points. We derived a number of Ehrenfest-type relationships, which are valuable in the discussion of the anomalous behaviour of $PrBa_2Cu_3O_6$, and some related systems.

Although it is of great venerability, the subject of fcc Fe thin films on the surface of copper has received new interest owing to the new pulsed laser deposition technique pioneerd in recent experiments. These new films exhibit a crystal structure very close to ideal layer by layer growth, which was not the case previously. We applied the fully relativistic spin polarized KKR method to study the orientation of magnetism in this films on the fcc(111) face of Cu. We found a reorientation transition at 2 monolayer, which is in excellent agreement with experiments. We also studied magnetic properties of Fe chains embedded

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[+] Permanent position: Budapest University of Technology and Economics

in Cu. Our results show that the (100) oriented chains have a magnetization perpendicular to the chain, while (110) oriented chains are magnetized along the chain.

We have investigated the transport properties of **unconventional condensates** in solids. The frequency dependent conductivity of spin density waves (SDW) has been determined in the presence of impurity scattering, and reasonable agreement with experiment has been found. We have established the theory of **unconventional SDW** by working out the thermodynamics and the optical properties of this system. Our results are expected to be relevant in a number of cases, when a robust thermodynamic phase transition is observed, but the order parameter can not be found by conventional means (hidden order). An example for this kind of system is the organic conductor α-$(ET)_2$, where we have successfully interpreted the measured threshold electric field in terms of our unconventional SDW model.

The transport in layered cuprates perpendicular to the CuO_2 planes is of great current interest due to possible non Fermi liquid behavior. We have calculated the out-of-plane optical response of **d-wave superconductors**[4], and explained the absence of the Drude peak by assuming coherent tunneling between the layers.

Copper-oxigen compound have strong electronic correlations. Upon doping a complex phase diagram develops with long-range antiferomagnetic order, magnetic fluctuations, charge and/or spin ordering, pseudogap type of behaviour, and superconductivity at temperatures up to 160 K. From the results of the electronic Raman scattering measurements we developed a phenomenological theory which describes the experimental results quantitatively in terms of a general metal-insulator transition.

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Attila Virosztek	viro@szfki.hu
Levente Vitos	lv@szfki.hu

Grants and international cooperations

OTKA T025505 Competition of ferromagnetism with other collective phenomena in the lattice models for electrons (P. Fazekas, 1998-2001)

OTKA T023390 Ab initio study of the structural stability of solids and surfaces (J. Kollár, 1997-2001)

OTKA T035043 Calculation of electronic states in metal- and oxide surfaces and nanostructures, (J. Kollár 2001-2004)

ESF Network program: Electronic structure calculations (J. Kollár, 1998-2002)

RTN Program Computational Magnetoelectronics (J. Kollár, 2000-2003)

DAAD-MÖB 2000/18 Spectroscopical properties of cuprates (I. Tüttő, 2000-2001)

AKP 2000-123 2,2 Quantum disorder and quantum critical behaviour in transition metal compounds (P. Fazekas, 2001-2002)

Publications

Articles

C.1. B. Magyari-Köpe*, L. Vitos, and J. Kollár: *Ab initio* study of structural and thermal properties of $ScAlO_3$ perovskite. *Phys. Rev.* **B63**, 104111/1-5 (2001)

C.2. L. Vitos: Total energy method based on the Exact Muffin-Tin Orbitals Theory. *Phys. Rev.* **B64**, 014107/1-11 (2001)

C.3. L. Vitos, I. A. Abrikosov*, and B. Johansson*: Anisotropic lattice distortions in random alloys from first-principles theory. *Phys. Rev. Lett.* **87**, 156401/1-4 (2001) Cover Picture from paper for Phys. Rev. Lett. **87**, (2001)

C.4. B. Magyari-Köpe*, L. Vitos, B. Johansson*, and J. Kollár: Parametrization of perovskite structures: an *ab initio* study. *Acta Cryst.* **B57**, 491-496 (2001)

C.5. A. Virosztek, B. Dóra* and K. Maki*: Microwave conductivity in spin density waves. *Ferroelectrics* **249**, 73-80 (2001)

C.6. B. Dóra*, A. Virosztek and K. Maki*: Threshold electric field in unconventional density waves. *Phys. Rev.* **B64**, 041101/1-3 (2001)

C.7. B. Dóra* and A. Virosztek: Thermodynamics and optical conductivity of unconventional spin density waves. *Eur. Phys. J* **B22**, 167-178 (2001)

C.8. B. Dóra*, K. Maki* and A. Virosztek: Out of plane optical conductivity in d-wave superconductors. *Europhys. Lett.* **55**, 847-853 (2001)

C.9. M. Opel*, R. Nemetschek*, F. Venturini*, R. Hackl*, I. Tütto, H. Berger*, L. Forró*, A. Erb*, B. Revaz*, E. Walker*: A Light-Scattering Study of Dynamical Carrier Properties in Cuprate Systems. *Ferroelectrics* **249**, 155-164 (2001)

C.10. L. Szunyogh*, B. Újfalussy, and P. Weinberger*: Magnetic anisotropy of ordered and disordered FePd thin films. *Phys. Rev.* **B63**, 184408/1-7 (2001)

C.11. J. S. Faulkner*, B. Újfalussy, N. Moghadam*, G. M. Stocks* and Yang Wang*: The mathematics of the polymorphous coherent potential approximation. *J. Phys.: Condens. Matter* **13,** 8573-8585 (2001)

C.12. I. Kézsmárki*, Sz. Csonka*, H. Berger*, L. Forró*, P. Fazekas, and G. Mihály*: Pressure dependence of the spin gap in $BaVS_3$. *Physical Review* **B63**, 081106/1-4 (2001).

C.13. B. Magyari-Köpe*, L. Vitos, B. Johansson*, and J. Kollár: Theoretical study of the high pressure structure of $ScAlO_3$ perovskite. *J. Geophys. Res.*, accepted for publication

C.14. A. Landa*, C-C. Chang*, P. N. Kumta*, L. Vitos, and I. A. Abrikosov*: Phase stability in stoichiometric and doped $LiMnO_2$: an *ab initio* study. *J. Electrochem. Soc.*, accepted for publication

C.15. L. Vitos, P. A. Korzhavyi* and B. Johansson*: Elastic property maps of austenitic stainless steels. *Phys. Rev. Letters*, accepted for publications

C.16. B. Magyari-Köpe*, L. Vitos, B. Johansson*, and J. Kollár: Model structure of perovskites: cubic-orthorhombic phase transition. *Comp. Mat. Sci.*, accepted for publication

C.17. B. Magyari-Köpe*, L. Vitos, G. Grimvall*, B. Johansson*, and J. Kollár: *Ab initio* study of the crystal structure of $CaSiO_3$ perovskite. *Phys. Rev. B*, accepted for publication

C.18. P. Fazekas, K. Penc, H. Berger*, L. Forró*, Sz. Csonka*, I. Kézsmárki*, and G. Mihály*: $BaVS_3$: from spin gap insulator to non Fermi liquid, *Physica B,* accepted for publication

Conference proceedings

C.19. A. Landa*, C-C. Chang*, P. N. Kumta*, B. Magyari-Köpe*, L. Vitos, R. Ahuja*, and I. A. Abrikosov*: First principles simulations of phase stability in stoichiometric and doped $LiMnO_2$. In: *Proc. Mat. Res. Soc. Symp.* Vol. 677, pp. AA6.16.1-AA6.16.6 (2001)

Book chapter

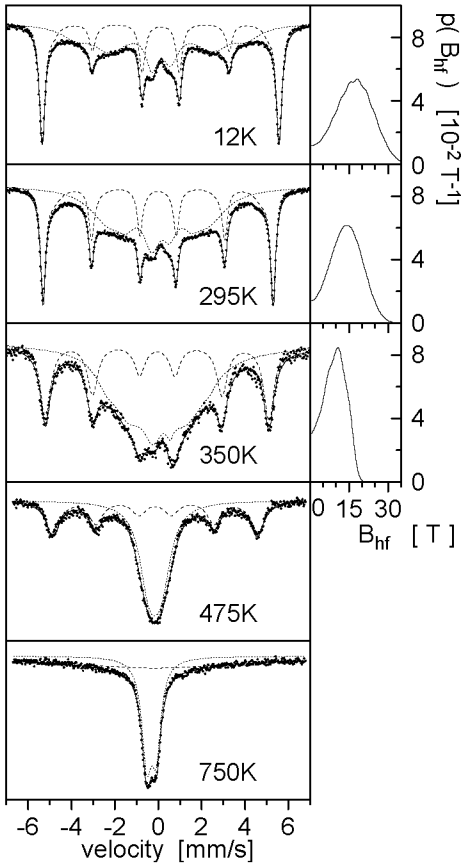
C.20. J. Kollár, L. Vitos, and B. Johansson*: *Ab initio* study of stability of surfaces and nanostructures. In: *Proc. Atomistic Aspects of Epitaxial Growth, Corfu 26-30 June, (2001)* NATO ASI Series, accepted for publication

See also A.7.

D. NON-EQUILIBRIUM ALLOYS

I. Vincze, J. Balogh, L. Bujdosó, D. Kaptás, T. Kemény, L.F. Kiss

Magnetic decoupling in nanocrystalline systems. — The role of exchange interaction between nanosize magnetic phases in composite systems or via nonmagnetic spacers in magnetic multilayers is a bone of contention for some time. Oscillatory dependence of the giant magnetoresistance on the thickness of the nonmagnetic interlayer spacer of magnetic multilayers and the shape of the magnetisation curves of such systems provide indirect evidences for the existence of an RKKY-type (Rudermann-Kittel-Kasuya-Yosida-type) exchange interaction between the ferromagnetic layers. Furthermore, increase of the Curie point in multilayers and that of the residual amorphous phase with respect to the precursor amorphous phase in Fe-Zr-B-Cu nanocrystalline alloys were also attributed to the effect of such interphase exchange interaction. However, absence of magnetic coupling between the ferromagnetic nanoparticles and the ferromagnetic residual amorphous phase is shown by the superparamagnetic relaxation in nc$Fe_{74}B_{18}Zr_7Cu_1$ observed via Mössbauer spectroscopy below $T_c^{res.am.}$. Superparamagnetic relaxation results in the broadening of the lines of the corresponding spectral components. In the case of nc$Fe_{74}B_{18}Zr_7Cu_1$ the bcc grains contain about 40% of the Fe atoms and the average geometrical size is 6.7 nm according to low temperature Mössbauer measurements and X-ray line broadening, respectively. $T_c^{res.am.}$ is less than 430 K as extrapolated from the temperature dependence of the average hyperfine field of the residual amorphous phase. However, the characteristic doublet of the paramagnetic amorphous phase can only be observed well above this temperature (e.g. 750 K), where the bcc contribution is almost completely smeared out because of the fast relaxation. At lower temperatures, but still above $T_c^{res.am.}$ (e.g. at 475 K) the effect of the fluctuating dipolar magnetic fields of the bcc grains can be seen in the spectrum of the residual amorphous phase as a significant line broadening. This fluctuation and the possible inhomogeneity due to some concentration gradient complicate the precise determination of $T_c^{res.am.}$. According to the Mössbauer measurements the superparamagnetic relaxation starts already above room temperature. It is illustrated in the figure for 350 K. Characteristic line broadening of the bcc components is observed although the residual amorphous phase is ferromagnetic with an average hyperfine field near to 10 T (corresponding to an average iron magnetic moment of 0.7-0.8 μ_B). It means that in this magnetically concentrated system the strength of the interphase exchange coupling does not exceed the magnitude of the dipolar field of the residual



Temperature dependence of the Mössbauer spectra of nanocrystalline $Fe_{74}B_{18}Zr_7Cu_1$. The full line is the fitted curve, dashed and dotted lines show the components of the bcc and the residual amorphous phase, respectively. The inserts show the hyperfine field distribution of the residual amorphous phase.

amorphous phase. At room temperature the estimated few kG dipolar field supresses the superparamagnetic relaxation of the bcc grains.

Atomic and magnetic structure of the interface in Fe/Ag multilayers. — Temperature dependence of the magnetic properties of Fe/Ag vacuum evaporated multilayers was studied in a wide range of layer thickness. The Fe/Ag multilayer samples were prepared by electron beam evaporation of the elements in a vacuum of 10^{-7} Pa. The samples studied contained Fe layers of nominal thickness, d_{Fe}= 0.2, 0.7, 1.4, 2.8, 5.6 and 11.2 nm with various Ag thickness, which was controlled by a vibrating-quartz oscillator. X-ray reflectivity peaks were observed on samples with Fe layer thickness $d_{Fe} \geq 1.4$ nm indicating the formation of continuous layers. For $d_{Fe} \geq 1.4$ nm the measured Mössbauer spectra can be attributed to ferromagnetic Fe layers, however, the hyperfine fields are significantly lower than that of pure α-Fe at elevated temperatures. It is attributed to a decrease of the Curie temperature due to Ag impurities in the Fe layers. Below 1 nm Fe thickness the formation of superparamagnetic particles was observed both by SQUID magnetization and by Mössbauer spectroscopy. The concentration dependence of the average hyperfine parameters is very similar to that published for co-deposited granular alloys where the increased low temperature hyperfine field and the apparently lower Curie temperature were attributed to the formation of non-equilibrium fcc $Fe_{1-x}Ag_x$ alloy. The magnetoresistance results could also be explained by the presence of small Fe clusters in the Ag matrix.

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Grants and international cooperations

OTKA T 030753 Magnetic systems with nanoscale inhomogeneities (I. Vincze, 1999-2002)

OTKA T031854 The influence of atomic volume and local environment to the anomalous magnetic properties of equiatomic alloys (T. Kemény, 2000-2003)

OTKA T034602 Magnetic properties of multilayers (J. Balogh, 2001-2004)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP9: Nation-wide co-operation for the study of non-equilibrium metallic materials (T. Kemény, 2000-2003)

Long term visitors

— Ass. Prof. Dr. Jan Dusza, D. Sc., Head of the Structural Ceramics Department, Institute of Materials Research, SAS, Slovakia 10.15.2001-11.15.2001 (KFKI-CMRC Grant, cooperation with Eötvös Univ.)

— Victorino Franco, D. Sc., associate lecturer, Dpto. Fisica de la Materia Condensada, ICMSE CSIC Univ. Sevilla, Sevilla, Spain, 10.10.2001-11.28.2001 (KFKI-CMRC Grant, host: L.F. Kiss)

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D.1. T. Kemény, D. Kaptás, L.F. Kiss, J. Balogh, I. Vincze, S. Szabó*, D.L. Beke*: Structure and magnetic properties of nanocrystalline soft ferromagnets. *Hyperfine Interactions* **130**, 181-219 (2000)

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See also F.1., H.5., I.1.

E. X-RAY DIFFRACTION

G. Faigel, G. Bortel, L. Gránásy, Z. Jurek, K. Kamarás, G. Oszlányi, S. Pekker, T. Pusztai, M. Tegze

Fullerenes and their compounds. — The fullerenes are closed shell molecules containing only carbon atoms. The most abundant among them is the C_{60} molecule. Even in the simplest form (i.e. solids of pure C_{60}) C_{60} is not fully understood. Illumination of the fcc pristine C_{60} by intensive light results in a phototransformation. This was the first case when intermolecular linkage of the fullerene molecules was proposed. After developing the production of C_{60}-photopolymer by solid state reaction, we introduced a novel method with a liquid phase transport of the monomer. Using this we increased the yield from the mg to the gram scale. This allowed the crystallization of the C_{120} cycloadduct dimer. X-ray powder diffraction revealed a face centered cubic structure with a=14.05 Å lattice constant, which can be well understood starting from the C_{60}-C_{60} intermolecular distance and a disorder of the dimer molecules in the lattice. Isolation of higher oligomers with the HPLC (High Performance Liquid Chromatography) technique is in progress.

We have also successfully prepared alkali and alkaline earth fulleride salts in order to systematically study the effects of molecular Jahn-Teller effect and crystal field on solid-state properties.

X-ray holography with atomic resolution. — In holography, the scattered radiation is mixed with a reference wave and the resulting interference pattern is recorded. The hologram contains both the intensity and the phase information and the 3 dimensional image of the object can be reconstructed. The most important limitation of this imaging technique is the spatial resolution, which is given by the wavelength and/or by the source size. Using x-rays for hologram forming and the atoms of the sample as sources or detectors, atomic resolution can be achieved. We were the first to demonstrate experimentally the feasibility of x-ray holography with atomic resolution in 1996. To make this technique usable in practice, we built an experimental setup at the European Synchrotron Radiation Source, and worked out the proper evaluation technique. Using this technique we could image the atomic environment of the Mn atoms in a PdMnAl quasi crystal. This was the first direct 3D imaging of the atomic decoration in quasi crystals.

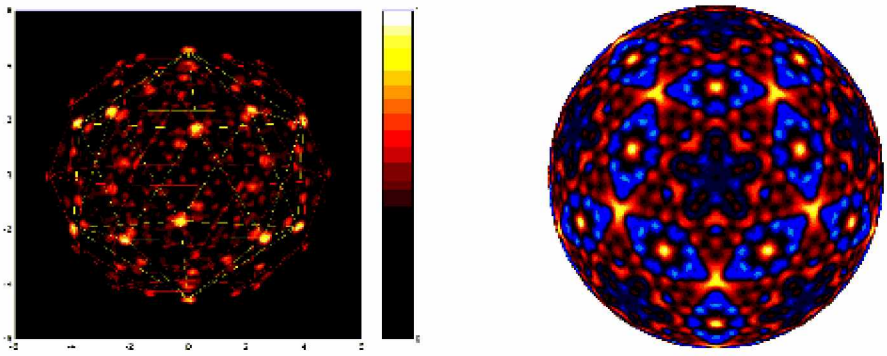

Fig.1. The atomic environment of the Mn atoms in a PdMnAl quasi crystal, (hologram right panel, reconstructed image left panel).

Theory of phase transformations. — Extending the work done in previous year, we performed a critical assessment of the classical kinetic approach to nucleation and growth. The

interfacial diffusion coefficient and the free energy of the glass-crystal interface have been evaluated via fitting the numerical solution of the kinetic equations to the nucleation rates and transient times measured on five stoichiometric oxide glasses. The interfacial diffusion coefficients obtained so were used to predict the macroscopic growth rates, which were compared with the respective experiments. For most of the compositions a good agreement is seen between experiment and theory. Differences amounting in two to four orders of magnitude were observed for the rest. The results depend only weakly on the cluster model used to relate the work of formation of clusters to the bulk interfacial and thermal properties.

We developed a phase field theory for binary crystal nucleation. In the one-component limit, quantitative agreement is achieved with computer simulations (Lennard-Jones system) and experiments (ice-water system) using model parameters evaluated from the free energy and thickness of the interface. The critical undercoolings predicted for Cu-Ni alloys accord with the measurements, and indicate homogeneous nucleation. The Kolmogorov-exponents deduced for dendritic solidification (Figure 2) and for ``soft-impingement'' of particles via diffusion fields are consistent with experiment. The calculations were performed on a cluster of 15 PCs by parallel processing.

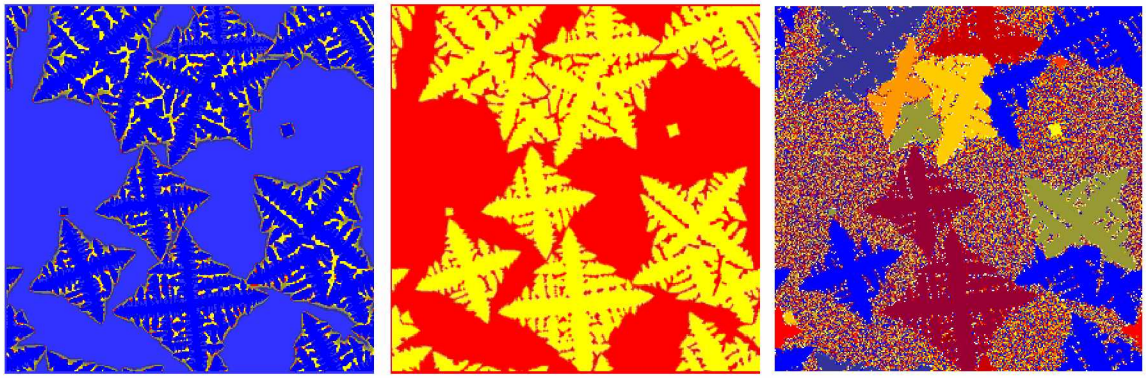

Figure 2. *Snapshots of two-dimensional phase-field simulation of crystal nucleation and dendritic growth in ideal binary alloy* (Ni-Cu) *at 1574 K and* $x = (c - c_s) / (c_l - c_s)$, *while* c_l *and* c_s *are the liquidus and solidus compositions, respectively. The pictures from left to right show the composition-, phase- and orientational fields. Black and white correspond to the liquidus and solidus compositions in the left panel and to the liquid and solid phases in the central panel, while the different gray tones stand for different crystallographic orientations in the right panel (orientation fluctuates in liquid).*

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Grants and international cooperations

OTKA T022041 Atomic resolution X-ray holography (M. Tegze, 2001-2004)

OTKA T025139 Theoretical investigation of the dynamics of nucleation and growth processes (L. Gránásy 1998-2001)
ESA[3] Prodex 14613/00/NL/SFe(IC), Modelling of Nucleation and Phase Selection (L. Gránásy, 2000-2003).
OTKA T029931 Structural studies of polymer fullerides (G. Faigel 1999-2002)
MTA – OTKA – NSF International Grant No. N31622 Research on the Optical Properties of Fullerenes (S. Pekker, K.Kamarás, D. B. Tanner* and A. F. Hebard* 1999-2001)
ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP8: Atomic level structural studies by photons and neutrons (Gy. Faigel, 2000-2003)
OTKA T 034198 Temperature and pressure dependent studies of the optical properties of fullerene salts (K. Kamarás, 2001-2004)

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[3] ESA = European Space Agency

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See also D.7., D.10., G.1.

F. ELECTRON CRYSTALS

G. Kriza, P. Matus[#], L. Németh[#], I. Pethes[#], B. Sas

Dissipation in high-critical-temperature superconductors. — The configuration and dynamics of vortices in Type-II superconductors play a vital role in the current carrying capacity of the materials. High-T_c superconductors such as $Bi_2Sr_2CaCu_2O_8$ (BSCCO) are special in this regard because of the very anisotropic electronic structure of this compound. We have investigated the onset of dissipation in BSCCO single crystals at low temperatures, in high magnetic fields and over long times (up to two weeks). We find that the threshold current for dissipation depends on the history of the sample: samples cooled in zero magnetic field exhibit a lower threshold current than those cooled in a high magnetic field. We observe that the field cooled (FC) preparation is metastable and relaxes towards a stable state close to the zero-field cooled preparation over a time scale of several days. The relaxation process is characterized as a function of temperature and magnetic field.

NMR in the novel high-T_c compound MgB_2. — One of the most significant discoveries of the year in the field of superconductors has been the observation of superconductivity in MgB_2 with an unusually high critical temperature 39 K. We have measured ^{11}B NMR spectra and spin-lattice relaxation rate in high quality isotopically pure samples of MgB_2. We have successfully interpreted a splitting of both the central and satellite transitions, not seen before in samples with natural abundance of the ^{11}B isotope, as arising from the spin-spin interaction of the boron nuclei.

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Grants and international cooperations

OTKA T023786	NMR investigation of collective electronic states in organic conductors (G. Kriza, 1997-2001)
OTKA T029877	Vortex motion in type-II superconductors (G. Kriza, 1999-2001)
TéT F-24/97	Periodic system in random field (B. Sas, 1998-2001, Hungarian-French Bilateral Science and Technology Cooperation)

Publications

Articles

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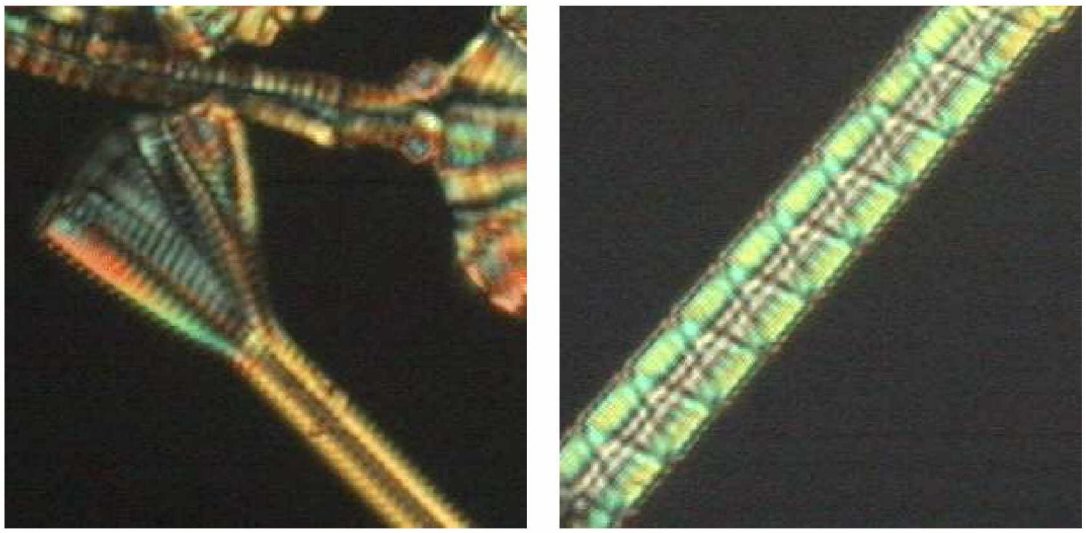
F.5. I. Pethes, B. Sas, G. Kriza, F. Portier*, F.I.B. Williams*, K. Vad*, S. Mészáros*: High-current differential resistance in $Bi_2Sr_2CaCu_2O_8$ single crystals. *Synthetic Metals* **120**, 1013-1014 (2001)

G. LIQUID CRYSTALS

Á. Buka, L. Bata, T. Börzsönyi, N. Éber, K. Fodor-Csorba, A. Jákli, I. Jánossy, Sz. Németh[#], T. Tóth-Katona, A. Vajda

A *synthetic method* has been developed for the preparation of new, five-ring, banana-shaped monomers. The substituents on the central ring are of high influence on the mesophase behaviour. The non-substituted compound has a B_2 phase below 100°C, the 4-chlororesorcinol derivatives have nematic phase, and the 2-methyl resorcinol compounds do not show any mesophase at all. The compound with B_2 phase forms chiral domains though it consists of achiral molecules. This compound is antiferroelectric with a tilt angle of 45 degrees yielding high contrast in electro-optic switching. The calamitic and banana shaped compounds were miscible in a narrow concentration range preserving their electro-optic switching ability.

The isotropic-smectic C phase boundary of a substance consisting of *non-chiral, banana-shaped molecules* shows patterns which clearly indicate the chiral structure of the more symmetric (smectic C) phase. The figures show polarizing microscopy images of a size of 0.1mm x 0.1mm.



The chiral structure is a result of two symmetry breaking processes originating from the polar ordering of the densely packed molecules and from the tilting of the plane of the molecules relative to the smectic layer normal.

Viscous fingering experiments in a radial Hele-Shaw cell have been performed using nematic liquid crystals as the more viscous fluid. The combined effect and the interplay between external and internal anisotropies have been detected and compared with phase field simulations. The inherent viscosity anisotropy of the system was regulated by an applied electric field while the external anisotropy was imposed by locally changing the capillary length. The finger velocity and its tip radius as a function of the anisotropies was measured and the behavior supported by the phase field model.

A complete morphology diagram of a *directionally solidified* nematic-smectic B growth front was established. In this large anisotropy system (presenting facets only in one direction) localized, drifting structures are formed near the Mullins-Sekerka threshold that

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can present stationary or oscillatory dynamics. To our best knowledge such phenomenon has never been observed before.

The spatial distribution of the azimuthal angles of the director has been determined for various *electroconvection patterns* — normal (NR), abnormal (AR) and CRAZY rolls — appearing in homeotropically aligned nematic liquid crystals at increasing voltages. The data obtained for the NR-AR transition correspond to a pitchfork bifurcation and are in quantitative agreement with theoretical predictions of the Ginzburg-Landau amplitude equations. At higher voltages the abnormal rolls may either form a (quasi)periodic domain structure of large wavelength or may be partially transformed into a spatially period doubled stacking of disclination loops (the CRAZY rolls).

A periodic modulation of the azimuthal angles was also found in another pattern of large wavelength — the prewavy pattern (PWP) — which appears at high frequencies below the electroconvection threshold. The voltage and frequency dependence of the basic characteristics of this pattern have been determined. The PWP often evolves into a defect free chevron structure which can be interpreted as a superposition of normal rolls onto the prewavy pattern.

The influence of *photoisomerization* on optical reorientation in *dye-doped nematic* liquid crystals was investigated. Special emphasis was placed on the effect of azo compounds with short *cis* lifetimes (milliseconds). A new method was developed to determine the non-linear absorption coefficients of the guest-host system.

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Grants and international cooperations

OTKA T-031808	Convective and interfacial instabilities in liquid crystals (Ágnes Buka, 2000-2003)
OTKA T-030401	Synthesis of aromatic and heteroaromatic liquid crystals and study of their physico-chemical properties (K. Fodor-Csorba, 1999-2002)
OTKA T-032667	Synthesis of low molar mass, monomeric and polymeric liquid crystals labeled by a stable isotope, and their spectroscopic studies (Katalin Fodor-Csorba, 2000-2003).
OTKA T-022772	Viscoelastic properties of smectic liquid crystals (Nándor Éber, 1997-2001)
OTKA T-023102	Investigation of physical properties of columnar and cubic mesophase (Antal Jákli, 1997-2001)
OTKA T-024098	Laser induced phenomena in smectic liquid crystals (István Jánossy, 1997-2001)

OTKA N-31165, MTA-OTKA-NSF (Hungarian-USA bilateral): Optical alignment of liquid crystals (István Jánossy, 1999-2001)

ERB FMRX-CT 96-0085) EC Research Network: Pattern formation, noise and spatio-temporal chaos (Ágnes Buka, 1996-2001)

IC15-CT98-0806 Inco Copernicus: Photonic devices: new liquid crystalline composite materials (István Jánossy, 1999-2001)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP11: Interaction of light with condensed matter (Nándor Éber, 2000-2003)

MTA-JSPS 39 (Hungarian-Japanese bilateral): Electrohydrodynamic instabilities and nonlinear phenomena in liquid crystals (Ágnes Buka, 1999-2001)

MÖB-DAAD (Hungarian-German bilateral): Liquid crystals of unconventional molecular structure (Ágnes Buka, 2000-2001)

MTA-INSA (Hungarian-Indian bilateral): Experimental and theoretical studies on liquid crystals (Nándor Éber, 2001-2003)

MTA-CAS (Hungarian-Chinese bilateral): Physical and chemical study of liquid crystals (Nándor Éber, 2001-2003)

MTA-SASA (Hungarian-Serbian bilateral): Structure and physical study of liquid crystals (Nándor Éber, 2001-2003)

MTA-WATWAW (Hungarian-Polish bilateral): Study of liquid crystals (Katalin Fodor-Csorba, 2001-2003)

MTA-ASCR (Hungarian-Czech bilateral): Synthesis and study of ferroelectric liquid crystals leading to preparation of mixtures with defined properties (Katalin Fodor-Csorba, 2001-2003)

MTA-CNR (Hungarian-Italian bilateral): New banana-shaped monomers and their polymer derivatives. (Katalin Fodor-Csorba, 2001-2003)

Long term visitors

— Erik Benkler, Darmstadt University of Technology, Darmstadt, Germany, 2x1 month, January, August (KFKI-CMRC grant, host: I. Jánossy)

— David Statman, Allegheny College, Meadville, Pennsylvania, USA, 1 September, 2001 -31 August, 2002 (Fullbright scholarship, host: I. Jánossy)

— Wojciech Otowski, Cracow University of Technology, Cracow, Poland, 1 October, 2001 -31 December, 2001 (KFKI-CMRC grant, host: Á. Buka)

Publications

Articles

G.1. T. Börzsönyi, T. Tóth Katona, Á. Buka, L. Gránásy: Regular dendritic patterns induced by non-local time-periodic forcing. *Phys. Rev. E.* **62**, 7817-7827 (2000).

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G.9. A. Jákli, G. G. Nair*, C. K. Lee*, L. C. Chien*: Electro-disclinic effect in tilted smectic phases of banana-shaped materials. *Liq. Cryst.* **28**, 489-494 (2001).

G.10. A. Buka, T. Börzsönyi, N. Éber, T. Tóth Katona: Patterns in the bulk and at the interface of liquid crystals. *Lecture Notes in Physics* **567**, 298-318 (2001).

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G.15. T. Börzsönyi, S. Akamatsu*, G. Faivre*: Dynamics of a faceted nematic-smectic B front in thin-sample directional solidification. *Phys. Rev. E.* accepted for publication.

G.16. D. Catalano*, M. Cifelli*, V. Domenici*, K. Fodor-Csorba, R. Richardson*, C.A. Veracini*: ^{2}H NMR and SAXS of a ferroelectric liquid crystal: Unwinding of the ferroelectric chiral helix by high magnetic fileds. *Chem. Phys. Lett.* accepted for publication.

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G.19. K. Fodor-Csorba, A. Vajda, G. Galli*, A. Jákli, D. Demus*, S. Holly*, E. Gács-Baitz*: Ester-type banana-shaped monomers and their electro-optical investigations. *Macromol. Chem. Phys.* accepted for publication.

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G.21. D. Z. Obadovic*, A. Vajda, M. Stancic*, S. Jovanovic-Santa*, J. Petrovic*, D. Lazar*: The synthesis of the chiral non-mesogenic D-seco estrone derivatives and their influence on the phase transitions of cholesteric liquid crystals. *Phase Transition* accepted for publication.

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G.22. T. Börzsönyi, S. Akamatsu*, G. Faivre*: Dynamics of a faceted nematic-smectic B front in thin-sample directional solidification. In: *Proceedings of the 4eme Rencontre du Non-Lineaire, Paris, 15-16 March 2001,* Eds.: Y. Pomeau, R. Libotta (NonLineaire Publications, Bat 510, Université de Paris Sud, 2001) pp.39-44, 2001.

Others

G.23. E. Mátyus, K. Fodor-Csorba, A. Jákli: New aspects (direction) of liquid crystal research area: banana shaped liquid crystal molecules. (In Hungarian) *Magyar Kémiai Folyóirat,* **107,** 227-234 (2001).

See also E.17., E.18.

H. METAL PHYSICS

K. Tompa, I. Bakonyi, P. Bánki, M. Bokor, Cs. Hargitai, Gy. Lasanda, L. Péter, J. Tóth, E. Tóth-Kádár

Metal-hydrogen systems. — In the ^{1}H NMR study of $\mathbf{Zr_yNi_{1-y}–H}$ amorphous alloy-hydrogen systems, the low temperature spin-lattice (T_1) relaxation time has been measured. The interpretation of T_1 concludes a strong paramagnetic contribution of unknown origin in the low temperature range. This result suggests the search of inhomogeneous echoes near the solid-echoes at very low temperatures, namely at 2-3 K range. The interpretation of the spin lattice relaxation time (T_1) and the shift terms (Knight and chemical shifts) are in progress, and the expected conclusions will reflect the electron structure of the system.

High purity $\mathbf{Pd_{1-x}Ag_x}$ (x=0.1; 0.2 and 0.35) alloys were charged with hydrogen, and NMR spectrum, T_1 and $T_{1\rho}$ spin-lattice relaxation time measurements in the laboratory and rotating reference systems were continued on this fcc crystalline alloy, a model material representing a chemically disordered system for hydrogen storage materials. In the very low temperature range (2-3 K), inhomogeneous echoes were detected near the commonly known solid echoes suggesting a strong paramagnetic contribution to the proton NMR spectrum of unknown origin. The free induction decay (FID) signal, moreover inhomogeneous echoes (detected at 0^0 phase) and mixed solid+inhomogeneous echoes (detected at 90^0 phase) at H/M=0.2 hydrogen content are shown in Fig. 1.

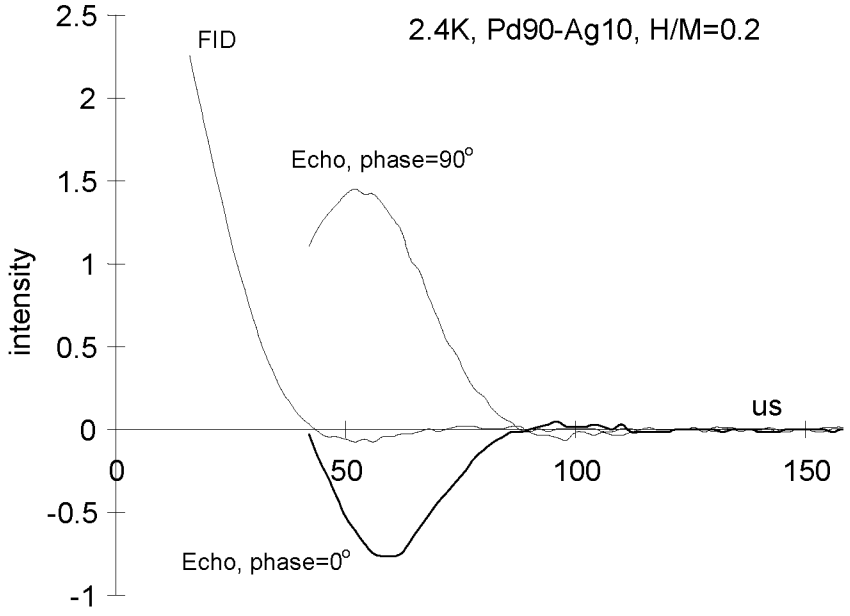

Figure 1. FID NMR signal and different echoes (see text) in a Pd-Ag-H alloy at 2.4 K

Using the electrolytic technology, the values of hydrogen concentration (c=H/M) measured by coulometry (c_F), significantly deviate from the results of other absolute measurements, that is $c_F \neq c$. The applicability of the Faraday law was examined in the hydrogen charging or discharging process of Pd metal. It was found that the resistivity ratio (R/R_0) versus (H/M) curves - where the hydrogen concentration was determined by the Faraday law - were "*consistently false*" if a certain common electrolytic pre-treatment was applied. The consistency means that $R/R_0(c_F)$ curves are independent of the value of the applied current density of charging (or discharging), so the main characteristics of the process of

hydrogenation are the same for a wide range of current density. A renormalized current density gives back the necessary $c_F = c$.

Looking for new fields of NMR research:

— **NMR on nanocrystalline copper.** — Quadrupole effects in the room temperature continuous wave ^{63}Cu NMR spectra, furthermore the shortening of the "$\pi/2$" pulse length and the echo amplitudes following two-pulse generation were investigated on nanocrystalline copper powders produced by cryogenic melting technique and by ball milling. Systematic measurements on the parent polycrystalline copper and on copper based Cu-Pd dilute alloys based on the same experimental basis were also made and the results are compared to that of the nanophase samples.

— **Cycloaddivity of carbon materials.** — New chemicals prepared from carbon materials (fullerenes and carbon nanotubes) by Diels-Alder type cycloaddition reactions were studied by NMR spectroscopy, namely by proton NMR spectrum and relaxation time measurements. The analysis showed that the applied reactants formed covalent bonds with the carbon materials. Parts (molecular groups) of the reaction products proved to be mobile i.e. undergoing reorientation motions on the basis of temperature dependent NMR measurements.

— **Nonlinear laser materials.** — Y-Al borates (YAB) were investigated by ^{11}B NMR spectroscopy, and quadrupole effects were used for the determination of boron location in polycrystalline and mono-crystalline samples. An illustration NMR spectra in Y-Al borates is shown in Fig. 2.

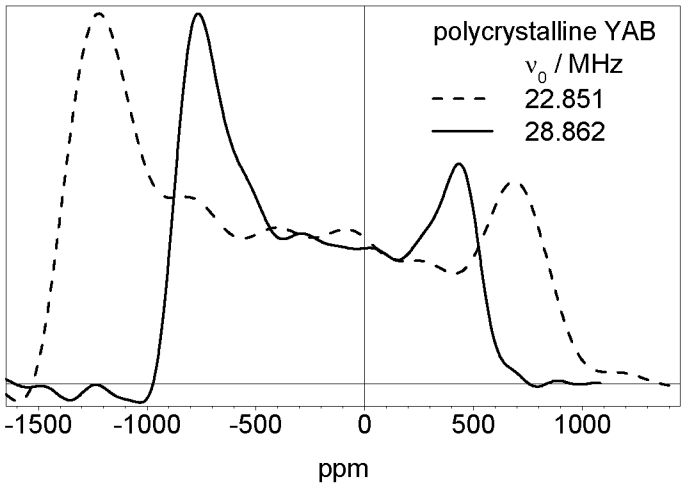

Figure 2. Quadrupole perturbed central component NMR spectra in Y-Al borates

Metastable metallic phases. — The microstructure and the average grain size were investigated by X-ray diffraction (XRD) and transmission electron microscopy (TEM) for nanocrystalline (n) Ni-P alloys obtained by annealing melt-quenched Ni-P amorphous alloys with 18, 19 and 22 at.% P. A detailed study of the nanocrystalline states obtained along different heat treatment routes has been performed: (i) $a \rightarrow n_i$: by isothermal annealing of the as-quenched amorphous alloys; (ii) $n_i \rightarrow n_{ii}$: by isothermal annealing of the nanocrystalline n_i state; (iii) $n_i \rightarrow n_{il}$: by linear heating of the n_i state. The heats evolved during the structural transformations were determined by differential scanning calorimetry (DSC). From these studies, a scheme of the structural transformations and their energetics was constructed, by including previous results on phases obtained by linear heating of the as-quenched

amorphous state of the same alloys. In estimating the grain boundary energies, in some cases it was necessary to assume a variation of the specific grain boundary energy during the phase transformation in order to understand the observed enthalpy and microstructure changes caused by the different heat treatments. As an important conclusion of the comparison of linear heating and isothermal annealing treatments, it is emphasized that the striking differences in the microstructural evolution along the two heating routes stem from the different time scales of the two types of experiments. This finding reinforces the importance of atomic diffusion processes (i.e., kinetics) in governing these structural transformations. Linear heating results in an energetically stable state with a high specific grain boundary energy and with grain sizes in the range 30-160 nm, and it yields a complete phase separation confirmed by the fact that the relative intensities of the XRD lines of each phase can be well described by the literature values. Isothermal annealing treatments, on the other hand, yield a nanocrystalline state with smaller grain sizes (10-40 nm) and a lower specific grain boundary energy. During the isothermal heat treatment, the precipitated Ni_3P grains may contain solute Ni atoms, while the fcc-Ni grains can be supersaturated in P atoms that is reflected by systematic changes in the XRD peak intensities. These observations lead to the conclusion that the microstructure and energetics of phases formed during structural transformations depend strongly on the routes along which the system is allowed to thermally evolve.

GMR in metallic multilayers. — Electrodeposited Co-Cu/Cu multilayers have been produced by two-pulse-plating from a $CoSO_4$ + $CuSO_4$ bath in order to investigate the influence of deposition conditions on the giant magnetoresistance (GMR) behaviour.

The influence of NaCl as an additive was studied for multilayers obtained under galvanostatic control. The addition of NaCl decreases the current efficiency of the multilayer deposition, and results in multilayers with lower GMR and higher electrical resistivity than the chloride-free bath. Structural studies performed by X-ray diffraction (XRD) and transmission electron microscopy (TEM) revealed that the grain size of the deposit and the degree of orientation also decreases if the additive is present. It has been concluded that the adsorption of chloride, the formation of copper(I) intermediate, the change in the deposition mechanism, the increase in nucleation rate and the occurence of a non-Faradaic current transient all contribute to the enhancement of the structural disorder that leads to the loss in GMR. It has been demonstrated that the presence of a component in the bath applied for the electrodeposition of magnetic multilayers can be critical for magnetoresistance properties. NaCl in as low as 0.5 mmol dm^{-3} concentration ($\approx$0.03 g/l) is capable of substantially modifying the properties of the resulting electrodeposited multilayers. It is believed that most of these effects are not specific to a particular additive but rather general for many agents used for d.c. baths. Baths used for pulsed electrodeposition of nanoscale magnetic/non-magnetic multilayers have to comply with a number of conditions quite different from those required for d.c. plating. First, the impurity level in the solution has to be well controlled. Second, the application of adsorbing, levelling or brightening additives commonly used in d.c.-plating has to be reinvestigated. Third, the negative ions in the salt of the metal to be deposited have to be inert and non-adsorbing like SO_4^{2-}.

A new electrochemical cell design with homogeneous current distribution was used to produce electrodeposited Co-Cu/Cu multilayers of 300 bilayer repeats from the two-component bath ($CoSO_4$, $CuSO_4$) with conventional potentiostatic/potentiostatic (P/P) and galvanostatic/galvanostatic (G/G) as well as unprecedented galvanostatic/potentiostatic (G/P) control. In contrast to common belief about the superiority of the P/P method, it was established that the specific deposition parameters rather than the deposition mode itself are decisive for the magnitude of the GMR effect. In experimenting for the optimization of the

GMR effect by varying deposition parameters such as the Co deposition current density and the Co- and Cu-layer thicknesses, the most favourable conditions extracted to obtain a pronounced GMR effect were found to be as follows: (1) large negative current density for Co deposition, e.g. –106 mA/cm^2, (2) a low negative potential for Cu deposition, e.g., -0.25 V, and (3) a relatively thick Cu layer, e.g. a nominal thickness of about 2 nm. Combining these parameters, a very distinct GMR peak is obtained in the G/P mode (Fig. 3). The magnitude of the GMR is at least 10 % at low fields of 1 kOe and hardly changes at higher magnetic fields.

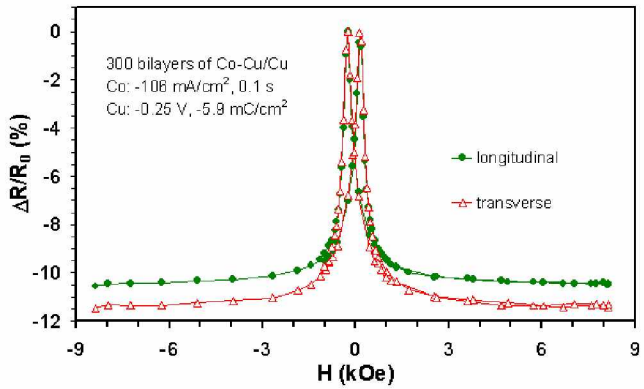

Fig. 3. Longitudinal and transverse magnetoresistance curves of electrodeposited Co-Cu/Cu multilayers prepared at optimized conditions in the G/P mode.

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Grants

OTKA T 031994	Random walk and diffusion of hydrogen in alloys (K. Tompa, 2000-2002)
OTKA F 032046	Preparation of metallic multilayers from compositionally modulated flowing electrolytes (L. Péter, 2000-2003)
OTKA D-38490	Study of potential hydrogen storage materials (M. Bokor, 2001-2002)
BAYATI[4]	Contract for "Diffusion and solubility study of hydrogen in IF steels" (L. Péter, 2001)

Long term visitors

— V. Weihnacht, Institute of Solid State and Materials Research, Dresden, Germany; May 7 – Aug. 4, 2001 (host: I. Bakonyi)

[4] BAYATI: Institute for Materials Science and Technology, Bay Zoltán Foundation for Applied Research

Publications

Articles

H.1. G. Lasanda, P. Bánki, K. Tompa: Hydrogen occupancy, ^{1}H NMR spectrum and second moment of Zr_XNi_{1-X}-H metallic glasses. *J. All. Comp.* **313**, 34-41 (2000); Erratum, *ibid.* **322**, 302 (2001)

H.2. Á. Cziráki*, I. Gerőcs*, M. Köteles*, A. Gábris*, L. Pogány, I. Bakonyi, Z. Klencsár*, A. Vértes*, S.K. De*, A. Barman*, M. Ghosh*, S. Biswas*, S. Chatterjee*, B. Arnold*, H.D. Bauer*, K. Wetzig*, C. Ulhaq-Bouillet*, V. Pierron-Bohnes*: Structural features of the La-Sr-Fe-Co-O system. *Eur. Phys. J B* **21**, 521-526 (2001)

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H.14. I. Bakonyi, J. Tóth, L. Goualou*, T. Becsei*, E. Tóth-Kádár, W. Schwarzacher*, G. Nabiyouni*: Giant magnetoresistance of electrodeposited $Ni_{81}Cu_{19}$/Cu multilayers. *J. Electrochem. Soc.*, accepted for publication

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See also: F.3., I.11, J.39.

I. METALLURGY AND MAGNETISM

L.K. Varga, I. Balogh, É. Fazakas[#], Zs. Gercsi, A. Kákay[#], P. Kamasa, G. Konczos, Gy. Kovács[+], J. Pádár, L. Pogány, F.I. Tóth, I. Varga

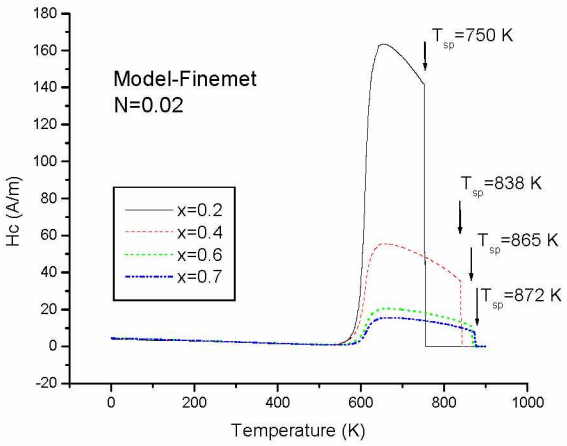
Soft magnetic nanocrystalline alloys. — To have a better understanding of the magnetic decoupling phenomena in two-phase soft magnetic nanocrystalline alloys, we have developed a new model to simulate the experimentally observed temperature evolution of the coercive field. We have taken into account the effect of dipole ferromagnetism, which starts to dominate the exchange ferromagnetism above the Curie temperature of the interphase region. This dipole ferromagnetism is a rather new concept and has an increasing importance in granular arrays used in MRAM's (regular artificial lattices) and in magnetic nanocomposites (disordered granular systems). The main concept can be formulated as follows: supposing a dipolar coupled nanogranular system, no ferromagnetic order will appear when the system can be reduced to a square lattice of point dipoles. But, both kinds of symmetry breaking, in the particle environment and particle shape, may favor ferromagnetic ordering. We suppose that the dipole ferromagnetism in a system of close-packed monodomain nanoparticles is sufficiently strong to replace the exchange interaction in averaging out the local anisotropy. The usual random anisotropy model (RAM) was applied for calculations, replacing the exchange stiffness constant, A, with a "dipolar" stiffness, A_d expressed rather heuristically in a mean field approximation as:

$$A_d = \frac{x\pi D^3}{54\mu_0} \cdot \frac{J_s^2}{D(x^{-1/3}-1)+a},$$

where D is the particle size, x is the crystalline fraction, J_s is the saturation polarization of the nanoparticle and *a* is the atomic distance.

The local anisotropy is dominated by the shape anisotropy expressed with the help of saturation polarization differences of the crystalline, J_S^{CR}, and amorphous, J_S^{AM}, component phases:

$$K_d = \frac{N}{2\mu_o}(J_S^{Cr} - J_s^{AM})^2 \bullet$$



The calculated evolution of the coercive field as a function of temperature is presented in Fig.1, which is a fairly good approximation of the experimentally observed values between the decoupling (T_c^{am}) and superparamagnetic transition temperatures (T_{sp}).

Fig.1. Model calculation of H_c for Finemet alloy.

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Using these fundamental results, a magnetic nanocomposite core was developed and tested for high frequency applications. This work was centered around the tasks of our NATO Science for Peace program aimed at preparing soft magnetic nanocomposites for audio and radio frequencies.

Scanning electron microscopy. — The JSM840 SEM facility has been equipped with a new LaB_6 cathode. This development necessitated also the renewal of the SEM vacuum system in order to ensure a vacuum of better than $5x10^{-7}$ Torr and the purchase of a new electronics control unit. This SEM modernisation improves the seconder electron contrast resolution from the previous value of 10 nm down to about 3 nm. Although to a different extent, the improvement of lateral resolution will have a beneficial effect in all aspects of SEM studies (surface morphology, magnetic domains, electron micropobe analysis) and also improves the sensitivity of such investigations. The increased resolution is especially significant at low electron energies and this is advantageous for studying the morphology of samples containing predominantly elements of lower atomic number (e.g., biological materials).

Combined thermal and magnetic analysis. — The evolution of amorphous Fe-based alloys during annealing takes place in many stages of reversible and irreversible transformations. New phases are formed at certain temperatures and may have first or second order character. Some processes are slower than the time of the experiment and it is not possible to establish criteria of equilibrium. In this case, the different heating rates produce different phases or some phases cannot be formed. The knowledge about the process is crucial to establish the heat treatment conditions to obtain expected phases. Besides monitoring the evolution of magnetic properties, thermal analysis is one of the most important method used to characterize structural phase transitions. While the precision measurement of the specific heat changes associated with structural transformations is possible using commercial DSC instruments, a simultaneous monitoring of the magnetic and thermal evolution is still not available. Combining a conventional thermomagnetic measurement with differential thermal analysis, we have developed an equipment for the measurement of changes in magnetic and thermal properties in one experiment.

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Grants and internationa cooperations

OTKA T-034 666	Iron-based bulk amorphous alloys and nanocomposites (L.K. Varga, 2001-2004)
OTKA T-035 278	Correlation between domain structure, dynamical magnetic properties and structural factors in soft magnetic equilibrium and metastable

alloys (2001-2004). The RISSPO is subcontractor (project leader: P. Kamasa) in this research grant of the Budapest University of Technology and Economics.

NATO Science for Peace Project 971930: Magnetic nanocomposites for transformer cores and magnetic refrigeration (L.K. Varga, 1999-2003)

OMFB grant "NATO 00002/99": Matching fund to NATO SfP Project 97/1930 (L.K. Varga, 1999-2002)

EU grant CRD2-2000-30349: Soft magnetic nanomaterials for high temperature and high frequency functional application in power electronic (L.K. Varga, 2001-2004)

NKFP3-00164/2001 Széchenyi NRP: Nanotechnology. (Participating scientist: L. Pogány, 2001-2003).

TéT E-9/2001 Preparation of new nanocomposite materials and their applications in materials engineering (L.K. Varga, 2001-2003, Hungarian-Spanish Bilateral Science and Technology Cooperation)

TéT F-36/00 Soft magentic nanocomposites: preparation, characterization and application in high-frequency power electronics (L.K. Varga, 2001-2002, Hungarian-French Bilateral Science and Technology Cooperation)

GE-TUNGSRAM: Contract for materials research by SEM (L. Pogány, 2001)

Long term visitors

— P.G. Bercoff, Universidad Nacional de Cordoba, Argentina; July 1 – 31, 2001 (host: L.K. Varga)

— D. Matveev, Institute of Solid State Physics of the Russian Academy of Sciences, Chernogolovka, Russia; July 2 – Aug. 2, 2001 (host: L.K. Varga)

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J. NEUTRON SPECTROSCOPY IN CONDENSED MATTER

L. Rosta, L. Almásy[#], M. Avdeev, L. Cser, J. Füzi, A. Len[#], E. Rétfalvi[#], L. Riecsánszky, Gy. Török

The Neutron Spectroscopy Department is one of the Laboratories of the associate Institutes forming the Budapest Neutron Centre, which operates the 10 MW Budapest Research Rector (BRR) and its experimental facilities on the KFKI site. This modern neutron source is open for the domestic and international user community and serves various tasks, such as basic and applied research in physics, chemistry, biology, materials science, as well as commercial utilisation and education. For neutron beam measurements different types of horizontal channels are available: seven thermal and two fast neutron channels; a tangential beam tube serves for the cold neutron guide system. Our Department on one hand operates several experimental stations located on the above beam-lines, on the other hand provides services for external users to perform experiments and exploit the obtained results. In year 2001 a major step in upgrading of the experimental possibilities was made: The new cold neutron research facility is in operation since February. This ensemble of equipment consists of the liquid hydrogen cold neutron source (CNS); the optimised supermirror neutron guide system and a set of experimental stations located in the neutron guide hall. The ensemble of the CNS and new guides provide an intensity gain of the order of 30-60. Besides this major instrument development programme, experiments were completed by the local staff and in collaboration with national or foreign users coming from university, industrial or other research laboratories.

We operate at BRR a pine-hole collimation type small angle scattering (SANS) instrument, a reflectometer (REFL) and a triple axis spectrometer (TAS) both installed on neutron guides. The installation of another TAS instrument is under way on a thermal neutron beam. Our activity related to neutron scattering is based essentially on experiments performed on the above spectrometers, some special studies, however, were performed at other neutron source facilities e.g. at ILL-Grenoble, HMI Berlin, PNPI Russia, or LLB Saclay (France) where we shared the construction of the Spin-Echo spectrometer (MESS).

The scientific activity of our team is focused on three major topics in condensed matter research, namely the investigation of structure and dynamics of *liquids* (e.g. various solutions, anisotropic fluids, biological based liquids), *soft materials* (gels, polymers, surfactants etc.) as well as materials properties of *solids* (metals, alloys, composites etc.). A considerable effort of our team is also devoted to fundamental problems of neutrons as well as the development of neutron scattering techniques.

Liquids. — Mixing properties of binary liquid solutions were investigated by different neutron scattering techniques. Small-angle scattering studies resulted in development of an effective method describing the structural properties of binary mixtures using thermodynamically measurable quantities and the value of the neutron scattering intensity at zero angles. By using the Kirkwood-Buff theory, the processes of the solute aggregation in various aqueous solutions have been revealed, and the macroscopically often hidden phase separation was measured on microscopic scale. The analysis of the measured concentration fluctuations results in the picture, that two co-existent sub-phases with different compositions are formed in the solutions. The dynamical behaviour of the components of the mixtures have been studied by quasi-elastic neutron scattering. The observed coupling between the motions of the solute and the solvent supports the hypothesis

[#] Ph.D. student

that the mechanism leading to the phase separation consists of a direct attractive interactions between the different types of molecules, and an effective attraction between the formed two-component microaggregates.

The combination of SANS and thermodynamic data allows one to calculate integrals of the pair correlation functions, which are otherwise not possible to obtain in a direct way. The Kirkwood-Buff integrals have been determined for aqueous solutions of several alcohols and methyl-substituted pyridines. These data can be used for checking the quality of the pair correlation functions, obtained from computer simulations or wide-angle scattering experiments.

Soft materials. — Interaction of DNA with poly(N-vinylpyrrolidone)-C_{60} complex (PVP+C_{60}) in D_2O has been studied by SANS at physiological temperatures T=20-40 °C to elucidate the mechanism of antiviral activity of fullerenes. Increasing the concentration of complex (C_C=0.1-1.0 %wt.) at a constant DNA content (C^* =0.1 % wt.), we observed a progressive complex association with DNA while the PVP revealed an opposite behaviour (maximum association degree at C~0.5 % wt.). Ability of complexes clustering with DNA (gyration radius of associates R_G ~ 15-30 nm) becomes more pronounced at 40°C as compared to ambient temperature.

Kinetics of ferrofluid ordering in the magnetic field and the decay of magnetic correlations of particles after field switching off have been investigated by neutron polarisation analysis. At ambient temperature, the long-time relaxation of magnetic scattering intensity $I_m \sim -\ln(t/\tau_L)$ with a time $\tau_L \sim 4 \cdot 10^7$s proves the existence of metastable clusters resembling structures in spin glasses. The local properties of the fluid with $CoFe_2O_4$-grains were examined in surface and interior layers by a thin neutron beam. We have found a specific magnetic correlation of particles, nearby the interface and free surface, inducing extra-magnetisation of surface regions extended to a few mm from the border to volume of ferrofluid.

Evaluation of magnetic flux distribution in ferrofluids has been performed by a new method, based on Larmor precession of neutron spin and Fourier analysis of precession phases over the neutron wavelength spectrum. Using this method for the thin layer of magnetic fluid in magnetic field (in plane), we detected an inhomogeneous distribution of induction which is stronger near the non magnetic fluid-metal interface. The surface layer covering ~60 % of the volume at low field H_1=10 Oe is shrunken to ~25 % at stronger field H_2=200 Oe when the fluid is substantially magnetised. Microscopic mechanisms of surface-induced ordering are discussed.

Chloroplast thylakoid membranes of higher plants form a highly stacked multilamellar system which is differentiated into granum and stroma regions. These membranes contain a great number of protein complexes embedded in the bilayer membranes which contains four major lipid components. During ontogeny, the membranes are self-assembled from the constituents that are produced in a concerted manner by the biosynthetic machinery. The structure and composition of the membranes also depend on the environmental conditions. Further, the mature membrane system exhibits a remarkable structural flexibility, and while keeping the integrity of the structure it is capable of undergoing substantial reorganisation upon changes in the environmental conditions: light intensity and temperature. The knowledge concerning the structure of the main components of the membranes have been advanced significally in the past decade, and for some components the near atomic resolution structural models have been presented. However, our understanding of the self-assembly of the complex membranes system, as well as the nature and mechanisms of the

structural rearrangements during the functioning of the membranes are still rudimentary. A small angle neutron scattering pattern of chloroplast thylakod membranes is shown in Fig.1.

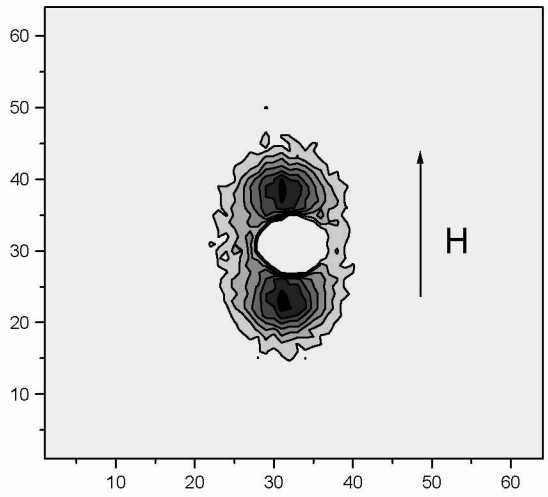

Figure 1. Small angle neutron scattering from the chloroplast thylakoid membranes, external magnetic field were applied (H=1.2T)

Solids. — According to the theoretical expectations, the potassium content in bubbles of sintered tungsten covers the internal surface forming a solid or liquid shell. Depending on the temperature, this coverage becomes thinner and thinner by rising the temperature, as more and more potassium from the shell evaporates into the gas phase in the center of the bubble. The two dimensional intensity distribution from SANS experiment enables to observe directly the morphology of potassium filled bubbles. This method has been applied to investigate the evolution of these bubbles at different temperatures. The tungsten wire samples, annealed at 2200K or 2400K include nearly spherical potassium filled bubbles. At lower temperature the potassium content in these bubbles is condensed in solid or liquid form covering the bubbles surface. Raising the temperature up to 1000-1020 K, the potassium coverage (shell) will disappear as the potassium forms dense gas phase in the bubbles at elevated temperatures. This is, however, a general theoretical model for describing the behavior of potassium at intermediate temperatures. There has been no experimental evidence published before to show this morphology. To compare the scattering intensities to the reference state of 1000K, differences in scattering intensities were analysed by using the model of hollow sphere. The results of the experiment correspond to the theoretical expectations.

Industrial application. — Neutron scattering experiments were performed at turbine blades, what are the main components of the axial compressor of a heavy-duty gas turbine. The structural material is a NiCrMoV steel usually adopted in the manufacturing of forged components for gas turbines. The bladed wheel experimented ~ 2500-peak cycles, with some 102% overspeed ones. In correspondence either of the same locations, or of some other reference points, measurement were performed in order to analyse the microstructure. The SANS experiment has shown different precipitate distribution examining different parts of the wheel.

Fundamental research using thermal neutron scattering. — Neutron standing waves (NSW) generated above a flat layer system during total external reflection has been observed and used for measuring and characterizing the depth profile of the layer structure under investigation. This non-destructive technique is particularly useful for measuring the thickness of buried layers. During the course of the experiment carried out in this year we used the above-mentioned phenomenon for calibration of the deposit rate of Ti by a

magnetron-sputtering machine. The layer system (estimated thickness of which is 1000 Å permalloy + 2000 Å Ti + 50 Å Gd + 100 Å Al) was deposited on a silicon wafer. The neutron scattering experiment was carried out using the reflectometer at the cold neutron source of BRR. Figure shows the small angle part (below Q = 0.025 $Å^{-1}$) of the measured neutron reflectivity on linear scale. Despite of the rather moderate resolution power, the minima related to the several first modes (2,3,4 and 5 marked by arrows in Fig.2.) of the NSW are clearly visible. The first order is hidden by the "blind spot" appearing due to the finite value of the collimation and the rather small length of the sample as well.

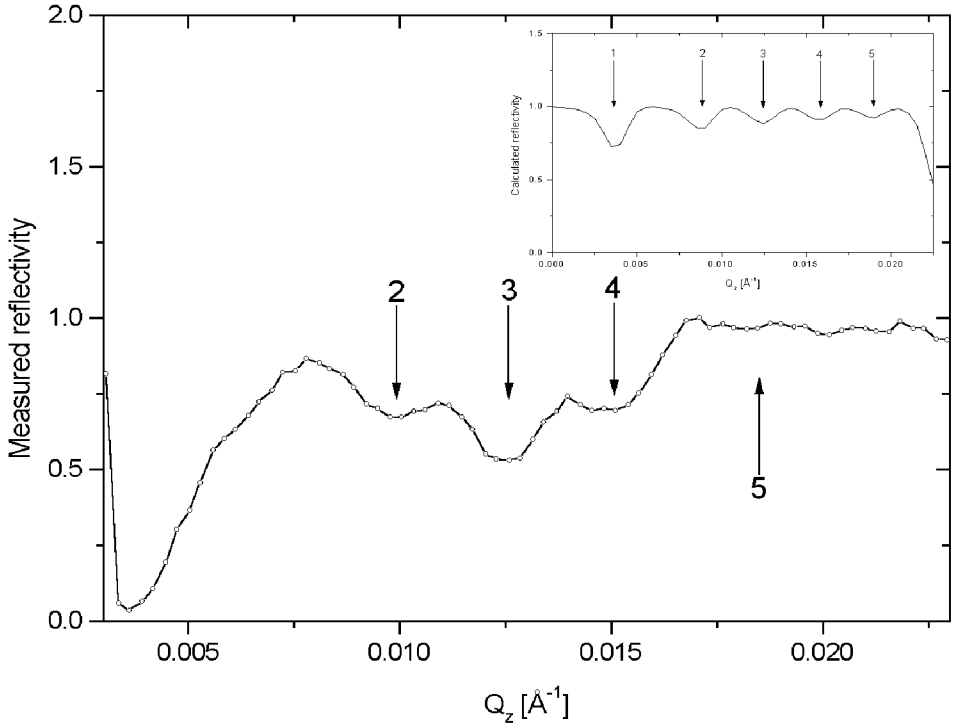

Figure 2. Several modes of a neutron standing wave in a reflectivity measurement

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Grants and international cooperations

EU ERB-CT96-0057 Perfect crystal neutron optics (L. Rosta, 1997-2001)
EU ERB-CT98-0098 Cold neutron optimisation (L. Rosta, 1998-2001)
EU ERB PL96-9007 Neutron Round Table (L. Rosta, 2001-2004)
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HPRI-CT-1999-00099 Acces to Research Infrastructure (BNC, L. Rosta, 2000-2002)

HPRI-1999-50016-CT European Polarized Neutron Initiative (Gy. Török 2000-2002)
IAEA B5-HUN/8879 Condensed matter research (L.Cser, 2000-2002)
OMFB 0478/97 High speed velocity selector development (L. Rosta, 1997-2001)
OMFB EU 097/97 Perfect crystal neutron optics (L. Rosta, 1997-2001)
OMFB EU-97-B4-98 Cold neutron optimisation (L. Rosta, 1998-2001)
OM –02617/1999 Large Area Neutron Detectors (L. Rosta, (2000-2002)
TÉT F-25/99 „Balaton" Neutron Detector Systems (L. Rosta 2000-2001)
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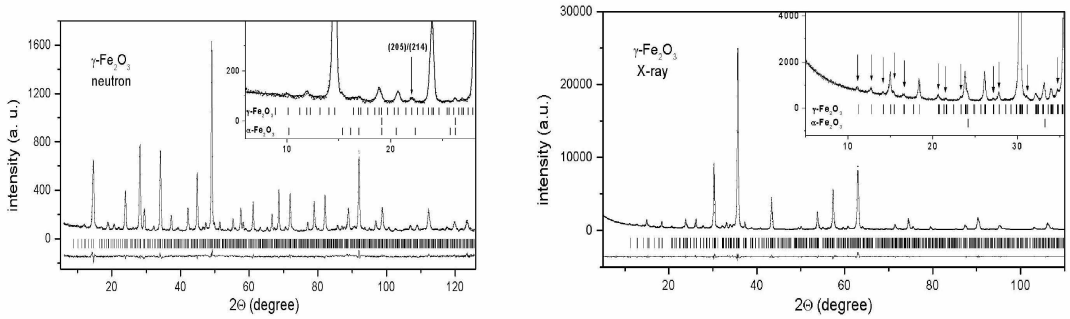
K. NEUTRON SCATTERING

E. Sváb, P. Jóvári, L. Kőszegi, Gy. Mészáros, L. Pusztai, Z. Somogyvári[#]

Nanocrystalline ferrites. — With recent advances in nanotechnology, **maghemite** (γ-Fe_2O_3) became of considerable interest for preparation of high-density recording media in magneto-optical devices. The structure of maghemite is closely related to that of the inverse spinel Fe_3O_4 but the network of iron atoms is partially depleted containing only ferric ions. We have performed a combined neutron and X-ray diffraction study on nanocrystalline sample with needle shaped grains of average size 240 nm x 30 nm, focusing our attention on the description of the crystallographic features of the correct space group, and the long range cation vacancy ordering. The experimental data were successfully fitted in space group $P4_12_12$ by multiprofile Rietveld method (Fig. 1). The refinement of the tetragonal unit cell parameters gave the values a=8.3498(1) and c=24.9960(6) Å, i. e. c/a=2.994(1), showing a slight distortion of the basic cubic lattice.



(a) *(b)*

Figure 1. (a) Neutron (λ=1.2251 Å) and (b) X-ray (Cu-Kα) diffraction pattern and Rietveld refinements of maghemite (γ-Fe_2O_3) in space group $P4_12_12$. The significant tetragonal extra reflections are indicated by arrows in the inserted enlarged figures.

It was established that remarkable changes occurred in the ordering of vacancies between the two types of octahedrally surrounded sites (8b and 4a), resulting in 82 % and 15% vacancy content, respectively. The corresponding first neighbour Fe_{4a}-O average distance decreased down to 2.01 Å, which is very similar to the distance of the other likewise occupied octahedral sites, while the polyhedron surrounding of the almost fully vacant Fe_{8b} expanded to an average first neighbour distance of 2.20 Å. A pronounced reduction in the ferrimagnetic sublattice moments was observed. These changes are attributed to nanosize-effect, as the published critical size determined from saturation magnetisation measurements for developing superparamagnetism is in the order of 40 nm.

Liquid and amorphous systems. — Structural aspects of two (of the very few) observed liquid-liquid phase transitions have been considered, via Reverse Monte Carlo (RMC) modelling of the corresponding experimental structure factors of liquid **sulphur** (*1-S*) and **phosphorus** (*1-P*). For *1-S*, it was found that although from a stand-alone data set, it is impossible to make the difference between S_8 rings and longer chains, from careful comparison of RMC structural models, it is evident that the lower temperature data corresponds to the presence of rings whereas at higher temperature, the presence of long

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chains is dominant. This finding means that finally, consistency between diffraction measurements and (text-book) explanation of this polymerisation (liquid-liquid) phase transition could be established. For *I-P*, the situation is somewhat more complicated: the lower pressure data can be described by P_4 molecules and the higher pressure data cannot, but this does not necessarily mean that at higher pressure, a true polymeric network would be formed.

As a continuation of our systematic structural studies on **molecular liquids**, we have measured by neutron diffraction the total structure factor of liquid **Si_2Cl_6**, **CBr_3D** and **CD_3I**. RMC modeling of these data confirmed our previous suggestion that reasonable structural models can be obtained on the basis of a single measurement if terminal atoms are relatively large and scattering from them dominates the diffraction pattern. In our cases, substitution of halide atoms by hydrogen/deuterium (in CBr_3D and CD_3I) led to increasingly unrealistic models.

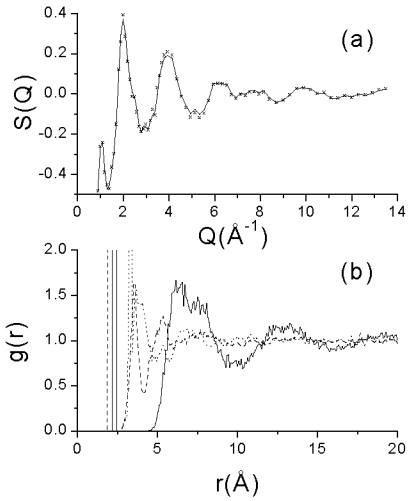

Figure 2. (a) Experimental (markers) and RMC simulated (solid line) structure factors for Si_2Cl_6. (b) Partial pair correlation functions calculated from the particle configurations. Solid line: $g_{SiSi}(r)$; dashed line: $g_{SiCl}(r)$; dotted line: $g_{ClCl}(r)$.

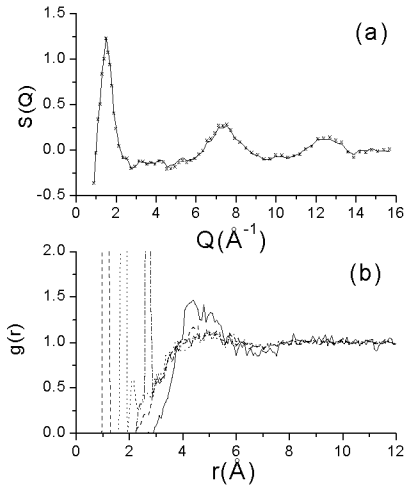

Figure 3. (a) Experimental (markers) and RMC simulated (solid line) structure factors for CD_3I. (b) Partial pair correlation functions calculated from the particle configurations. Solid line: $g_{CD}(r)$; dashed line: $g_{ID}(r)$; dotted line: $g_{DD}(r)$; dash-dotted line: $g_{CC}(r)$.

By RMC modeling of neutron and X-ray diffraction data on **molten $ZnCl_2$ and $MgCl_2$**, we showed that although the structures are similar in terms of two-body correlations, there are important differences in the higher order correlations (e.g. bond angle distributions). It was therefore possible to demonstrate that there is a structural basis for the high viscosity and good glass-forming ability of molten $ZnCl_2$, and why this is not the same for $MgCl_2$.

Internal stress studies. — Internal stresses play an important role in the lifetime of engineering materials. Binary alloys, where the two components have different linear thermal coefficients are under investigations by high resolution neutron diffraction. For $Fe_{95}Cu_5$ it was found, that after special heat treatment, Cu precipitates first on the grain boundaries of iron matrix and the remaining Cu — at lower temperature — precipitates inside the grains. The inside Cu suffers higher stresses than the ones on the grain boundaries.

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Grants and international cooperations

OTKA T 029402 Neutron diffraction study and modelling of partially ordered systems (E. Sváb, 1999-2002)

OTKA T 029433 Dynamic neutron-, gamma-, and x-ray radiography investigations and modelling of streaming processes (sub-contract E. Sváb, 1999-2002)

OTKA T 32308 Neutron diffraction at the Budapest Research Reactor (L. Pusztai, 2000-2003)

EU HPRI-CT-1999-50013 Software for computer Aided Neutron Scattering (L. Pusztai, 2000-2002)

NWO N 31766 Polarised neutron investigations of nanocrystalline materials (L. Pusztai, 2000-2002)

AKP 2000-92,4 Interpretation of diffraction data from molecular liquids (L. Pusztai, 2001-2002)

HAS-BAS (Hungarian-Bulgarian bilateral) Project N15: Structure study by neutron scattering (E. Sváb, 1999-)

HAS-SRA (Hungarian-Swedish bilateral): Neutron diffraction study of molecular liquids (L. Pusztai, 2001)

HAS-MMST (Hungarian-Mexican bilateral): Reverse Monte Carlo simulations (L. Pusztai, 2001-)

Long term visitor

— Kiril Krezhov, Institute for Nuclear Research and Nuclear Energy, Bulgarian Academy of Sciences, April 3-May 15 and November 3-December 15, 2001 (Host: E. Sváb)

Publications

Articles

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L. INTERACTIONS OF INTENSE LASER FIELDS WITH MATTER

Gy. Farkas, S. Varró and, I. Bányász

Experimental research. — In the course of our experimental activities aiming the construction of a superintense table top Nd:glass laser system, we have realized a passive mode–locked and Q–switched generator unit delivering ultrashort bandwidth–limited laser master pulses of 2 picosecond duration at 1 Hz repetition rate. These 0.1 mJ energy pulses have been then stretched by an optical grating pair arrangement. The stretched pulses entered a special regenerative amplifier and after achieving several mJ energy were coupled out by a pulse selector. In the next step the streched and amplified pulses have been anplified further in an amplifier chain containing the end amplifier unit. At the end the high–energy pulses were compressed to a couple of picosecond duration again by another grating pair, resulting very high ($> 10^{15}$ W/cm^2) light intensities.

In addition, we have produced transmission gratings in planar waveguides via electron and ion beams, and built temporal holograms via spectral hole burning.

Theoretical research. — We have given a detailed analysis of the electromagnetic field configuration inside plasmas generated by ultrashort strong laser pulses. The radiation due to the nonrelativistic motion of the electrons in the overdense region has been considered the main part of high harmonics, whose polarization dependence on the incoming fundamental beam has been treated to explain the the experimentally observed polarization properties.

By refining our earlier approach, we gave a theoretical interpretation of our recent experiments which demonstrated that high energy x-ray fields of about 10-20 keV photon energy may be generated by irradiating a gold target with laser light at grazing incidence to create a surface plasma by applying, in addition, a strong static negative voltage to the metal plate.

By considering a laser-induced oscillating double layer along the surface of a metal and its action on an electron of the metal, a theoretical analysis of recent experiments on infrared photoemission from metal surfaces has been given with results fitting quite well with the measured data. We have generalized the double–layer potential model beyond the dipole approximation concerning the interaction of the metallic electrons with the high–intensity laser field.

Concerning a fundamental theoretical problem, we were able to construct the Wigner functions of zero angular momentum eigenstates of free particles in 2–, 3– and higher N–dimensions in closed analytic form. Theses results give a deeper insight into the nature of the recently discovered so–called “quantum anti–centrifugal force” in 2-dimensional motion.

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Grants and international cooperations

OTKA T032375 Experimental and theoretical investigation of new fundamental physical processes (laser-matter interactions) induced by laser beams of superintense, 10^{15}-10^{20} W/cm^2 laser systems. (Gy. Farkas, 2000-2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP11: Interaction of light with condensed matter (N. Éber, 2000-2003)

TéT – F-3/00 (Hungarian-French Bilateral): Application of x-ray sources in the „femtosecond" regime. (Gy. Farkas, 2001-2002)

TéT –D-41/00 (Hungarian-German Bilateral): Study of laser-induced nonlinear processes in thin solid films. (S. Varró, 2001-2002)

Long term visitors

— Uwe Schwengelbeck, Universitat Bielefeld, Bielefeld, Germany, April, 2001. (host: S. Varró).

— Cyril Bonnefoy, Ecole Politechnique, Paris, France, July, 2001. (host: Gy. Farkas).

Publications

Articles

L1. K. Gál* and S. Varró: Polarization properties of high harmonics generated on solid surfaces. *Optics Communication* **198**, 419-431 (2001)

L2. I. Bányász: On the semi-physical developing effect of the AAC developer on holograms recorded in Agfa-Gevaert 8E75HD emulsions. *Optics Communications* **192**, 27-35, (2001)

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M. LASER PHYSICS

K. Rózsa, G. Bánó[#], L. Csillag, Z. Donkó, P. Hartmann[#], P. Horváth[#], Z.Gy. Horváth, M. Jánossy, K. Kutasi[#], P. Mezei

Atmospheric pressure glow discarge. — In previous experiments the cross-section of the positive column and the current density as function of pressure were studied at the two ends of the column in air, N, and He glow discharges using copper electrodes, in the pressure range of 100-760 torr. The cross-section and the current density were observed to be different at the two ends, except for a narrow pressure range around 200 torr. A gas discharge model has been developed, which took into account the appearance of dissociative recombination of molecular ions. On the basis of this model, the pressure dependent current densities were given at the two ends of the positive column. At the cathode end, at the border of the Faraday dark space, because of the presence of fast electrons originating from the cathode region, the current density could be connected to the cathodic one. The other end of the column is at the border of the anode space, where the current density is determined by the anode fall and the electron mobility. The numerical results received from the model were found to be in sufficient agreement with experiments in the case of air. However, since data on the pressure dependence of the anode fall have not been reported for other gases, the numerical calculations could not be carried out for N and He gases. The agreement of our model with the results of measurements obtained in air makes it probable, however, that the similar behavior of the positive columns observed in the case of N and He can also be explained by our model.

Gas laser studies. — Within the framework of metal ion laser research a new type of high voltage discharge is tested recently. As most of the metal ion lasers are pumped by charge transfer reaction between nobel gas ions and metal atoms, a high density of both species must be present in the active region. The idea of the hollow anode-cathode arrangement of the electrodes, originally developed for sputtered metal ion lasers, is now combined with thermal evaporation of the metal. This way the discharge current and the metal vapour density can be controlled independently. Parametric studies of the small signal gain and the output power were carried out for the blue transitions of the $He\text{-}Zn^+$ laser system. The possibility of light amplification on the 210 nm transition of the zinc ion will be investigated in the near future.

Plasma experiments and modelling. — The effect of the secondary electron emission coefficient on the voltage-current-pressure characteristics of glow discharges has been investigated. A simulation model was developed for helium glow discharges in a wide pressure range (1-100 mbar). The model includes the formation of He_2^+ molecular ions, and several plasma reactions between ground-state and excited atoms, atomic and molecular ions. Charged particle bilayer systems (where pointlike charges interacting through Coulomb potential are located in two separate quasi-two-dimensional layers) have also been investigated. Our molecular dynamics simulations showed sequence of structural phase transitions induced by changing of the layer separation. We developed a Monte Carlo simulation code to investigate the properties of classical, strongly coupled electron – hole bilayers, and studied the localization (caging) of particles in three-dimensional one-component plasmas.

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Grants and international cooperations

NATO SfP 971989	High beam quality UV lasers for Microelectronics (K.Rózsa, 1999-2004)
OMFB 01553/99	High beam quality UV lasers for Microelectronics (K.Rózsa, 1999-2004)
OTKA T - 25941	Ultraviolet lasers in controllable-temperature hollow cathode discharge (K.Rózsa, 1998-2001)
OTKA T - 25989	Numerical modeling of gas discharge plasmas (Z.Donkó, 1998-2001)
OTKA F - 25503	Hollow cathode discharges and lasers in gold vapor (G.Bánó, 1998-2001)
OTKA T - 34156	Modern plasma simulation techniques (Z.Donkó, 2001-2004)
OTKA T- 29112	Excitation processes in electrolyte cathode glow discharge (P.Mezei , 1999-2002)
IKTA-00178/2000	Digital imaging spectroellypsometrical quality control arrangement (Z.Gy.Horváth, 2001-2004)

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M.6. P. Mezei, T. Cserfalvi*, M. Jánossy: On the pressure dependence of the positive column cross section in high pressure glow discharges. *J. Phys. D: Appl. Phys.* **34,** 1914-1918 (2001)

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N. FEMTOSECOND LASERS

R. Szipőcs, S. Lakó, K. Szőcs

Optical thin-films in femtosecond laser systems. — Continuing our research started in 1993, dispersive dielectric mirrors were developed for different femtosecond laser systems such as: (a) ion-beam-sputtered (IBS) multi-cavity Gires-Tournois mirrors (MCGTI) for mode-locked, mirror-dispersion-controlled, diode pumped Cr:LISAF lasers operating at University of St. Andrews (Scotland) and ICS Trieste and (b) ultrabroadband chirped mirrors (CM) for optical parametric amplifiers (OPA) in collaboration with R&D Lézer-Optika Bt., Hungary, and MLD Technologies, USA. The MCGTI mirrors exhibit reflectivities R > 99.97% and negative group delay dispersion of -100±10 fs^2 over a bandwidth of 780 to 880 nm. Dispersive properties of MCGTI mirrors originate from coupled resonances in multiple $\lambda/2$ cavities embedded in the layer structure. Alternatively, the design of our ultrabroadband CM-s developed for the OPA system was obtained by our novel spatial frequency domain optimization technique. The mirrors exhibit high reflectivity and a constant group delay dispersion over bandwidths of 210 THz and 140 THz, respectively, allowing sub-5-fs pulse generation in the visible with the OPA laser system built at the University of Tokyo. A similar mirror set in combination with a deformable mirror device was developed for a tunable visible OPA system delivering tunable 7 fs pulses at the University of Toronto.

Pulse compression in microstructure (photonic crystal) optical fibers. — In collaboration with Bell Laboratory of Lucent Technologies Inc. (USA), researchers from the University of Szeged (Szeged, Hungary) and R&D Lézer-Optika Bt., the possibility of femtosecond pulse compression in microstructure optical fibers were investigated both theoretically and experimentally. Femtosecond pulses with energies of 1 nJ and time durations of 150 fs from our tunable, 76 MHz Ti:sapphire laser oscillator operating at around 750 nm were used for our studies. The length of the pulses can be compressed to one tenth by applying our high Δn, single mode microstructure optical fiber exhibiting zero group delay dispersion at 767 nm, and by proper extracavity dispersion compensation. Our experimental results fit well to computer simulation results, which are based on our theoretical model developed for describing the nonlinear pulse propagation in the optical fiber. The model comprises the reduced form of the differential equation that worked correctly for modeling fs pulse optical parametric oscillators. We are convinced that our proposed simple "upgrade" of 100 fs pulse laser oscillators will help to considerably reduce the temporal resolution of ultrafast measurements in many ultrafast spectroscopy laboratories.

Femtosecond time resolved spectroscopy using a pump-probe setup. — In collaboration with Lucent Technologies, USA, a femtosecond pump-probe experimental setup has been developed for time resolved spectroscopy of chemical, biological and medical samples. The setup comprises a synchronous viola/blue pump pulse for excitation and a white light continuum probe pulse for transient absorption measurements over the 450..1100 nm wavelength regime. The tunable 100 fs pumpe pulses are obtained by second-harmonic-generation of our tunable 100 fs NIR pulses generated by our Ti:sapphire oscillator "FemtoRose 100 TUN" in a BBO crystal. The continuum is generated in a relatively long (ca. 12 cm long) piece of Lucent Technologies special microstructure optical fiber. Samples for our studies were obtained from several different academic institutions and universities located in Budapest or Pécs.

Sub-micrometer pulse train machining of diamond like carbon layers. — We fabricated sub-micrometer holes on 100 nm diamond like amorphous carbon (DLC) coated surfaces by ablation with femtosecond laser pulse trains of a Ti:sapphire laser oscillator. In the case of DLC coating on Si wafer, one order of magnitude less than the focal spot, sub-micrometer damaged area could be achieved due to nonlinear processes.

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Grant

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O. METAL OPTICS

Z. Szentirmay, A. Hoffmann, N. Kroó, Z. Lenkefi

Installation of an STM/AFM microscope. — In order to study the surface morphological behaviour of vacuum deposited metal (as e.g. Ag, Au, Pd) and dielectric film (fullerenes) a new, Russian made, NT-MDT type P47 surface probe microscope with STM and AFM heads was purchased at the end of the last year. During the concerned time interval testing and checking processes were made. Numerous problems appeared with the software and with the electronics, those, however, seem to have been eliminated by now.

Investigation of laser evaporated gold/silver films. — Scanning tunnelling microscope measurements were performed with a 4-way apparatus (i.e. topography, current, thermionic and thermal images) on thermally evaporated Au films which were covered (decorated) with laser deposited Ag films of 0,5 - 2 nm thickness. Measurements were made both with tungsten, gold and silver tips changing by these the chemical potential between the layer and tip. With the help of this technique it became evident that the crater like structure on the topographic images was built during the laser evaporation. Also, thermionic pictures proved that near the center of the craters silver fragments should always exist, more or less sunk into the basic gold film. Preparation of additional AFM images of these samples is in progress.

Charge density waves in photorefractive crystals. — Since March 2001 one of our colleagues has been working as postdoc fellow in the Heinrich-Hertz-Foundation at the University of Bonn, Germany. His task is to construct STM head for the measurement of the decay of charge density waves in photorefractiv dielectrics, e.g. BiGeO. On the basis of his earlier activity he makes optical, electronic and software developments, too.

Fabrication of tunnel tips. — For tunnel microscopic investigation we successfully solved the problem of fabrication of silver and Pt/Ir tunnel tips, which can not be purchased commercially. Silver and Pt-20%Ir alloy wires of 0.25 mm diameter and specially controlled electrochemical etching were used which resulted tips with $r<50$ nm radius of sufficiently high output. In both cases the preparation methods differ substantially from those published earlier.

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P. LASER APPLICATION

A. Czitrovszky, P. Jani, M. Füle[#], H. Jancovius, I. Kertész, Á. Kiss, M. Koós, Z. Lipp[#], A. Nagy, I. Pócsik, M. Veres[#]

Optical measuring techniques. — A new forward-backward laser scattering method was developed for the sizing, counting and the estimation of the complex refractive index of aerosol particles in the sub-micron and micron size-range, in collaboration with the University of Vienna. For the modeling of this method a new algorithm was proposed, and for the data evaluation a new software was created.

A measuring head, based on the above mentioned method was constructed and calibrated for various particles. The results show a number of benefits of the new method in comparison with the previous airborne counting methods.

Work in the field of integrated optical sensor for the revelation of laser radiation, its presence and direction of propagation has been finished. Theoretical work has been done for the study of the statistics of scattered intensities. Findings of the computational model were proved by experiments. Technical criteria of sensors have been specified.

A new nuclear airborne particle counter with a modular measuring head was developed with increased sensitivity, better signal/noise ratio and improved signal evaluation system. In the frame of EU COLOSS program this equipment was installed in large-scale nuclear accident simulation experiment facility. The measurement of the hot nuclear aerosols released from LWR fuel rods heated up to 2200°C show new relations between the aerosol concentration, its size distribution and steam concentration during the experiment.

The mechanical and electronical system of a differential particle mobility analyzer was constructed.

A measuring system for the standardless determination of the quantum efficiency of photon counting detectors using entangled photon pairs was developed. This method was applied for measuring the absolute quantum efficiency of different quantrons.

Solid state laser development. — Further development and application of Er:glass laser was continued. The optimization of the operating parameters and increasing the repetition rate was achieved.

In collaboration with GE LIGHTING a cutting technology for combined different coils was developed using a laser system based on a Nd:YAG laser. This technology was optimized for different cutting conditions.

Amorphous carbon layers. — Photoluminescence (PL) investigations of a-C:H thin layers prepared either from methane or benzene source gases were performed with the aim of specifying the whole range of light emitted by these samples that contributes considerably to a further understanding of the fine structure of the electron density of states and the details of the radiative recombination in this material. We have shown composite feature of PL spectra, consisting of numerous characteristic bands, some of these already appear in the visible range of excitation, the others can be excited by UV light only. Three peaks with maximum position in the range of 4.34 – 4.50 eV, 3.93 – 4.01 eV and 3.64-3.70 eV are in the ultraviolet region. Additional peaks appear in the region of 3.17 – 3.22 eV and 2.85 – 2.92 eV beside the well-known broad PL band with maximum in the 2.1 – 2.33 eV range. The relative intensity of new bands varies on deposition conditions. Our results measured

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on numerous samples strongly suggest the existence of some type of intrinsic radiative centers.

The growth process of the carbon film was followed by IR spectra, by investigating film prepared under different deposition conditions. Surprisingly good spectral resolution could be achieved on samples deposited from benzene as source gas at relatively high pressure and low voltage conditions. Because the C-H bond-stretching region contains intensive aromatic components, we draw the conclusion, that the benzene ring structure can survive the deposition condition in the plasma, the ionization could eliminate hydrogen atom from the molecule. The structure will probably have a high active surface, what might have practical application possibilities.

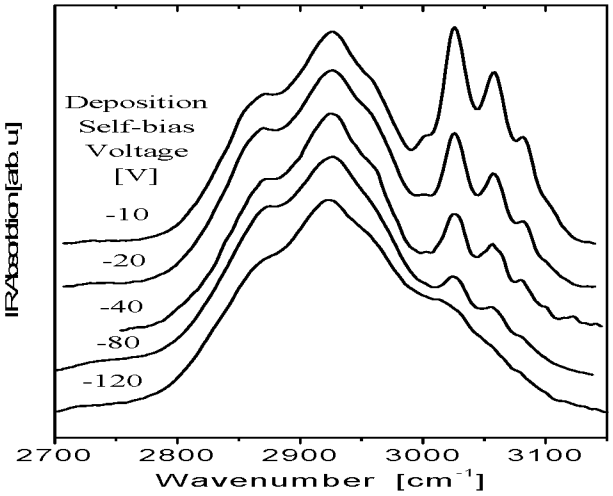

Fig. 1. C-H stretching region of the infrared spectra of hydrogenated amorphous carbon deposited at 400 mtorr under the listed selfbias voltages from benzene vapour.

Optical strength of a-C:H thin layers was investigated under influence of UV laser pulses in the ns and fs region at two different laser wavelengths. The possible utilization of these films in laser and microelectronic technology motivates these studies. The damaged area was found to depend linearly on the laser fluence in a narrow region around the damage threshold tested by rising number of pulses and fluence. The 2 – 3 times higher optical damage threshold for fs pulses on both wavelengths used, can be explained by the different weights of electronic and thermal processes in case of strongly different pulse lengths. Accumulative effects for multiple pulse impact were detected which were more clearly developed for UV region. The incubation process was the shortest for long pulse lengths.

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Grants and international cooperations

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OMFB 00887/99 Development of the DMA for the determination of the electrical charge of nuclear aerosol particles (A. Czitrovszky, 1999-2001)

OMFB 02126/99 Integrated optical sensor for the revelation of laser radiation, its presence and direction of propagation (P. Jani 1999-2001)

GE – SZFKI No 472/2000 Development of cutting technology for Wo-Mo coils (I. Kertész 2000-2001)

TéT-A24/2000 (Austro-Hungarian Bilateral): Development of dual wavelength particle counter (A. Czitrovszky, 2000-2001)

NATO SfP-973849 Carbon as Materials for Electrochemical Storage of Energy (I. Pócsik, 1999-2003)

OTKA T-026073 Electronic states, charge carrier localization and their interaction with the structure in amorphous carbon films (M. Koós, 1998-2000)

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See also N.5., N.7.

Q. OPTICAL THIN FILMS

K. Ferencz

Optical thin film structures in femtosecond laser systems. — We have continued our research concerning the development of dispersive dielectric mirrors for different femtosecond laser systems such as low-loss chirped mirrors for mode-locked Ti:sapphire laser oscillators, BBO based parametric oscillators and high power femtosecond Ti:sapphire laser amplifiers. Special ultrabroadband chirped mirrors have been developed for pulse compression experiments at the Technical University of Vienna, Austria. The pulse duration of the compressed pulses is below 5 fs. Using the high power compressed pulses of the commonly developed Ti:sapphire amplifier system built at the TU Vienna, coherent X-ray emission was investigated from a laser induced He plasma in the water window. The aim of the present development is generation of X-ray radiation having higher power, which makes it possible for practical applications such as X-ray microscopy and microlithography. Special X-ray filter sets were developed for these applications. Tilted-front-interface chirped mirror technique have been developed for the reduction of the fluctuations of the group delay dispersion of the conventional chirped mirrors in the frame of the cooperation between TU Wien and the Research Institute for Solid State Physics and Optics.

Other developments on optical coatings. — Our work on optical waveguides deposited on optical gratings is still in progress for optical sensors used for medical applications. We started basic experiments in nanobiotechnological application of optical waveguides. We investigated the effect of surface relief grating on the morphology and waveguiding properties of the deposited dielectric layers. Transparent electrodes were developed for porous silicon light emitters. Special interference filters were developed for high sensitivity detection of protein molecules elaborated by gene manipulation methods.

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Contract

OPTILAB-SZFKI No 364 Nanobiologycal application of optical thin films (Kárpát Ferencz, 2001)

Publications

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Q.2. G. Tempea*, V. Yakovlev*, B. Bacovic*, F. Krausz*, K. Ferencz: Tilted-front-interface chirped mirrors. *J. Opt. Soc. Am. B* **18**, 1747-1750 (2001)

R. GROWTH AND CHARACTERIZATION OF OPTICAL CRYSTALS

I. Földvári, L. Bencs, E. Beregi, V. Horváth, Á. Péter, K. Polgár, O. Szakács, Z. Szaller

Growth and study of nonlinear borate crystals. — The post-growth degradation and the chemical stability of borate crystals such as BaB_2O_4 (BBO), LiB_3O_5 (LBO), $CsLiB_6O_{10}$ (CLBO) and $Li_2B_4O_7$ (LTB) crystals were followed in relation to the growth conditions, structural defect content, and the surface preparation methods. Close connection was found between the hydration induced degradation process and the structural defect content of the crystals. Surface defects caused by mechanical operations promote hydration.

Planar waveguide was prepared in lithium tetraborate $Li_2B_4O_7$ crystal by 2 MeV helium implantation. It was established that the optical properties of the guiding core are not affected by the implantation process. The produced defects are isotropic and localized at the optical barrier without extension towards the surface. Optical losses are less than 2 dB/cm.

Er-doped $YAl_3(BO_3)_4$ (YAB) single crystals were successfully grown by the top-seeded flux method. The first detailed absorption spectra of Er in YAB single crystals were measured in the 220-1600 nm spectral region between RT and 10 K. The energy levels and Stark components of 12 transitions from the $^4I_{15/2}$ ground state were identified. The number and shape of the spectral lines suggest that the Er^{3+} ions are built into one specific lattice site (yttrium positions) without aggregation at high dopant concentrations (0.12 Er atoms /YAB mole). The nonlinear YAB crystal with homogeneous, high Er-content is a good candidate for self-frequency-doubling laser.

The solid phase synthesis of $RGa_3(BO_3)_4$ (R = rare earth) type compounds was studied starting from R_2O_3:$3Ga_2O_3$:$4B_2O_3$ mixtures. The dominant structures produced in the 575-1050°C range depended on the specific rare earth. In the case of La and Nd, $R(BO_2)_3$ type metaborates, intermediate RBO_3 and $GaBO_3$ borates were formed. In the series from Sm to Er the $RGa_3(BO_3)_4$ huntite borates were formed through intermediate RBO_3 and $GaBO_3$ products. It was first shown the formation of dolomite type $YbGa(BO_3)_2$ double borate.

Growth and study of stoichiometric $LiNbO_3$ single crystals. — A series of DSC and X-ray diffraction measurements were performed in order to establish proper chemical and thermal conditions for the formation of the stoichiometric material. From these results we concluded that the growth temperature is the key parameter, which determines the composition of the crystal. Below a certain temperature threshold (about 1114°C) the growing crystal is stoichiometric, independently from the K_2O content in the high temperature top seeded solution growth technique (HTTSSG). This threshold limits the choice of other solvents for the growth of stoichiometric $LiNbO_3$ single crystals.

Low temperature luminescence spectra of stoichiometric Cr:$LiNbO_3$ and congruent Cr,Mg:$LiNbO_3$ were determined. Cr^{3+} impurity occupy preferentially Li^+ sites in the crystal lattice, while in Mg co-doped crystals Cr^{3+} on Nb^{5+} sites are also present. Under high hydrostatic pressure a transformation of the dominant Cr centers occurs from low- field state to high field state. The measured shift of the luminescent lines correlated well with the theoretical estimations.

Growth and study of bismuth tellurite crystals. — The oxidative and reductive processes in the Bi_2TeO_5 / Bi_2TeO_6 system were followed by thermoanalytical methods. Using powdered Bi_2TeO_5 samples, the oxidation starts at about 450°C but complete oxidation can

only be achieved by long annealing of the samples in oxygen ambient at 670°C. At higher temperatures the Bi_2TeO_6 decomposes. Above 790°C the loss of TeO_2 is also evident. With the regular thermoanalytical heating rates (2-10°C/min) the oxidation and reduction sections overlap each other. Using combined mass spectrometric and thermoanalytical investigations it was shown, that starting from pre-prepared Bi_2TeO_6, the decomposition begins at about 670°C and, loosing oxygen, the Bi_2TeO_5 composition is restored by 860°C. The oxidation rate of Bi_2TeO_5 single crystals is extremely low, and the thermal treatment destroys only a thin surface layer of the samples. Thus, the oxidation and subsequent reduction do not influence the bulk quality of the single crystals grown from the melt and slowly cooled down to room temperature during the growth.

Bi_2TeO_5 single crystals were implanted with 800 keV Au^+ ions at RT. Strong absorption was observed in the 600-630 nm range after annealing the samples between 500 and 700°C, indicating the formation of gold nanoclusters. The average radii of the Au colloids were estimated to be 3-4 nm. Studies using RBS/channeling technique indicated that full recrystallization of the samples could not be achieved in the annealing temperature range used.

Analytical spectroscopic investigation of oxide and borate crystals. — $LiBO_2$ assisted melt-digestion technique was developed to get proper solution from YAB crystals for spectroscopic investigations. Atomic absorption spectroscopy (AAS) and inductively coupled plasma optical emission spectrometric (ICP-OES) methods were developed to determine the real composition (Y, Al, B main components), dopant concentration (Ce, Cr, Dy, Er, Yb) and impurity level (Mo from the flux applied) of YAB crystals.

The AAS method with transversally heated graphite atomizer (THGA) was improved for Cr and Cu dopants of Bi_2TeO_5 crystal samples. The proper alteration of the atomization conditions (i.e. use of chemical modifiers, application of mini-flow of the internal furnace gas during atomization, and use of end capped graphite tubes) has led to more reliable analytical results.

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Grants and international cooperations

OTKA T-034176	Growth and study of nonlinear optical crystals and crystal structures (K.Polgár, 2001-4)
OTKA T-032339	Optimization of the parameters of the acousto-optic tunable filters (L. Jakab (BME) and Á. Péter, 2000-2003)
OTKA T-029756	Growth and complex study of bismuth tellurite single crystals (I. Földvári, 1999-2002)
OTKA T026619	Application of spectrochemical methods for crystal growth studies. (T. Kántor (ELTE) and L. Bencs, 1998-2001)

OTKA T 024091 Growth and study of nonlinear optical crystals transparent in the far UV region (K. Polgár, 1997-2001)
ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP12: Growth and complex study of optical crystals (J. Janszky and I. Földvári)
OM-DDKKK 00004/2000 R & D Centre, Nonlinear Optics department (I. Sántha (PTE) and Á. Péter, 2001-2003).
OM FKFP 30/2000. Research Project Investigation of the formation process of complex rare-earth borates by thermoanalytical and X-ray diffraction methods. (J. Madarász (BME) and E. Beregi, 2000-2002)
OM-TÉT D-2/99 Hungarian-German bilateral R&D project: Improvement of the analog volume holographic recording technique (I. Földvári, 2000-2002)
COST Action P2. Application of nonlinear optical phenomena: Project WG1/1. Materials and systems for optical data storage (I. Földvári, 1998-2001)
Project WG2/4. Nonlinear optics for quantum communication (K. Polgár, 1998-2001)

Publications:

Articles

R.1. J. Madarász*, E. Beregi, J. Sztatisz*, I. Földvári and G. Pokol*: Combined DTA and XRD study of sintering steps towards $YAl_3(BO_3)_4$. *J. Thermal Anal. & Calorimetry* **64,** 1059-65 (2001)

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R.3. A. Boudrioua*, C. Bakhouya*, J.C. Loulergue*, P. Moretti*, K. Polgár: Low-loss optical planar waveguides in $Li_2B_4O_7$ crystals formed by He^+ implantation. *J. Appl. Phys,* **89**, 7716-21 (2001).

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R.5. A. Kling*, M.F. da Silva*, J.C. Soares*, P.F.P. Fichtner*, L. Amaral*, F.C. Zawislak*, I. Földvári, Á. Péter: Gold nanoclusters formed by ion implantation into Bi_2TeO_5. *Nucl. Instr. Meth. Phys. Res. B.* **175-177** (2001) 331-4

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R.13. A. Kling[*], M.F. da Silva[*], J.C. Soares[*], P.F.P. Fichtner[*], L. Amaral[*], F.C. Zawislak[*], I. Földvári, Á. Péter: Gold nanoclusters formed by ion implantation into Bi_2TeO_5. In: *Proc. of Mat. Res. Soc. Fall Meeting, Boston, November 2000*, **647** (2001) pp. 05.14.1-05.14.6 (Mat. Res. Soc.)

R.14. I. Földvári, C. Denz[*], J. Petter[*], F. Visinka[*], Á. Péter: Progress in hologram writing in Bi_2TeO_5 single crystals. In: *Proc. Nonlinear Optics for the Information Society NOIS, Third Annual Meeting of the Cost Action P2, Enschede October 26-28, 2000),* Ed: A. Driessen, Kluwer Publ., accepted for publication

R.15. N. Kukhtarev[*], T. Kukhtareva[*], V. Edwards[*], L. Mager[*], A. Fort[*], M. Rbino[*], I. Földvári, D. Frazier[*], B. Penn[*], H. Abdeldayem[*] and T. Hudson[*]: Volume and surface phase holographic gratings in the photorefractive crystals. In: *Proc. COST P2, Budapest, 16-19 May 2001*, Ed: Y. Lion, Europian Union, Brussel, accepted for publication

Book chapter

R.16. I. Földvári, Á. Péter: Growth and properties of Bi_2TeO_5. In: *Encyclopedia of Materials: Science and Technology.* Vol. 6. Ed. S. Mahajan, Pergamon Press, Amsterdam, 2001. Chapter: 5.30. pp. 512-5.

See also: S.7., S.11., S.12., S.13., S.18.

S. CHARACTERIZATION AND POINT DEFECT STUDIES OF OPTICAL CRYSTALS

A. Watterich, G. Corradi, E. Hartmann, L. Kovács, K. Lengyel[#], L. Malicskó, G. Mandula

Characterization of optical crystals. — The electrical conductivity of congruent and quasi-stoichiometric $LiNbO_3$ crystals was measured in the temperature range of 150-300 °C using dc method. The activation energy of congruent crystals was higher (1.11±0.03 eV) than that of quasi-stoichiometric ones (0.96±0.3 eV). The type of doping ions (Mn or Fe) did not affect the activation energy.

Dislocation motion in NaCl(Pb) crystals with and without magnetic field was investigated in cooperation with Russian coworkers: the dislocation mobility decreased when the crystals were deformed in magnetic field.

Microscopy and IR spectroscopy of laser damages. — Connection between OH^- impurities (present generally in melt-grown oxide crystals) and structural laser-damages microscopically observable in photorefractive Fe:$LiNbO_3$ crystals was expected. Indeed, by comparative FTIR spectroscopic studies of defect-sensitive OH^- bands in $LiNbO_3$ crystal samples of same origins and different histories the appearance of an OH^- band at ~3507 cm^{-1} was observed in Fe-doped Y-cut samples as a result of laser irradiation. This refers to an irradiation induced rearrangement of hydroxyl ions via proton migration, probably leading to laser-promoted formation of special Fe^{2+}_{Li}-OH^--Fe^{3+}_{Nb} point defect complexes. These defects seem to be nanoscale damage traces preceding the microscopically observable structural laser-damages.

Thermal fixing of holographic gratings in $LiNbO_3$. — Holographic scattering was introduced as a technique to determine the activation energy for thermal fixing of refractive index patterns in photorefractive crystals. After recording a parasitic hologram at ambient temperature, the time dependence of the transmitted intensity was determined at the fixing temperature. The temperature dependence of the time constant allowed us to evaluate the thermal activation energy. The activation energy was determined in congruent and nearly stoichiometric $LiNbO_3$ crystals doped with Mn or Fe, respectively ($E_a \approx 1.02 - 1.25$ eV). The obtained values were compared with those determined employing the two-wave mixing and DC conductivity measurement techniques. The method of holographic scattering is much simpler then two-wave mixing technique and gives the same results at high density of compensating ions. At low free ions concentration, it is an ideal sensitive technique to detect the possible dependence of the compensation time constant on the spatial frequency and to determine the concentration of free ions that are responsible for thermal fixing. The results are in agreement with those obtained from the kinetics of OH^- ions which has the perspective to provide site-specific information on hydrogen defects responsible for the thermal fixing process.

Point defects in oxide crystals. — UV illumination at 77 K was efficient at producing Vo' and $Vo^{\bullet}$ centers (three and one electrons captured at an oxygen vacancy, respectively) in electron-irradiated TeO_2 samples. The concentration of the Vo' center could be reduced drastically by illumination with light between 500-650 nm. Similar studies of optical absorption at low temperature have indicated a broad band at ~600 nm which is due to the Vo' center. The above processes are explained with the assumption of the presence of a

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diamagnetic Vo^{x} center (two electrons at an oxygen vacancy). UV light removes an electron from a Vo^{x} center yielding a $Vo^{\bullet}$ center, and the free electron will be captured by another Vo^{x} center resulting in a Vo' center. The reverse process takes place either by heating the crystal or illuminating it with 600-nm light in the absorption band of Vo'; an electron will be liberated from the Vo' center yielding a Vo^{x} center and the free electron will be recaptured by a $Vo^{\bullet}$ center increasing the concentration of diamagnetic Vo^{x} centers.

Point defects in stoichiometric $LiNbO_3$ single crystals. — Mobile intrinsic Nb^{4+}-type electron polarons induced by pulsed laser or electron beams have been shown to get trapped at remaining antisite Nb defects (Nb on Li site) even in high purity nearly stoichiometric $LiNbO_3$ crystals, in parallel with the presence of a pronounced photorefractive response in such crystals. These effects can be strongly reduced by further improving stoichiometry beyond the 99.95 mol% limit, thereby diminishing the concentration of antisites below that of the charge carriers and other defects. This will be useful e. g. for non-linear optical and real-time holographic applications. Improving stoichiometry, recombination luminescence acquires a longer component not observed for non-stoichiometric compositions where luminescence appears only on the nanosecond scale, the decay of bound polarons mostly occurring in a radiationless process. Site-selective excitation-emission spectroscopy of Er^{3+} in closely stoichiometric $LiNbO_3$ crystals revealed the same Li incorporation sites as for lower Li content, showing that charge compensation requires defects of the same intrinsic type in all cases.

X-ray storage phosphors. — EPR, photoluminescence and photostimulated luminescence studies were carried out in Eu^{2+} doped fluorobromozirconate glass ceramics and $BaBr_2$ single crystals before and following X-irradiation. Electron and hole trapping processes underlying X-ray image recording and stimulated detrapping processes used for luminescent readout have been characterized. Orthorombic $BaBr_2$ nanocrystal inclusions prepared by appropriate annealing procedures in the glass ceramics were shown to be essential for the existence of photostimulated luminescence. The corresponding recombination processes in other phases including the glassy phase itself turned out to be radiationless and of no use for X-ray imaging applications.

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Grants and international cooperations

OTKA T 022859	Determination of the structure of point defects by spectroscopic, conductivity and quantum chemical methods. (A. Watterich, 1997-2001)
OTKA T 023092	Characterization of multicomponent nonlinear optical crystals. (E. Hartmann, 1997-2001)
OTKA T 026088	Fundamental processes of hologram fixing in photorefractive crystals. (L. Kovács, 1998-2001)

OTKA T 034262 Investigation and optimization of crystalline and glassy systems for data processing (G. Corradi, 2001-2004)
OTKA T035044 Gyulai-Tarján school in crystal physics (E. Hartmann, 2001-2004).
ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP12: Growth and complex study of optical crystals (A. Watterich, 2000-2003)
TéT German-Hungarian Intergovernmental S&T Project, D 6/98 Characterisation of optoelectronic oxide crystals with advanced spectroscopic methods (G. Corradi, 1999-2001)
HAS – Bulgarian Academy of Sciences joint project (No. 36): Growth and characterization of oxide crystals for optical application (L. Kovács, 2000-2003)
HAS – CNR (Italy) joint project (No. 4): Growth and complex characterization of rare-earth doped crystals for photonics (L. Kovács, 2001-2003)
HAS-Polish Academy of Sciences joint project: Structure of real crystals (A. Watterich, 1999-2001)
HAS- Russian Academy of Sciences joint project (No. 22.): Mechanical properties of oxid and ionic crystals (E. Hartmann, 1999-2001).

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Articles

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S.2. M.A. Ellabban*, G. Mandula, M. Fally*, R.A. Rupp*, L. Kovács: Holographic scattering as a technique to determine the activation energy for thermal fixing in photorefractive materials. *Applied Physics Letters*, **78**, 844-846, 2001.

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S.6. S. Schweizer*, G. Corradi, A. Edgar* and J.-M. Spaeth*: EPR of Eu^{2+} in fluorobromozirconate glass ceramics. *J. Phys.: Condens. Matter,* **13**, 2331-38 (2001)

S.7. L. Grigorjeva*, V. Pankratov*, D. Millers*, G. Corradi, K. Polgár: Transient absorption and luminescence of $LiNbO_3$ and $KNbO_3$. *Integrated Ferroelectrics* **35**, 1867-79 (2001)

S.8. A. Baraldi*, R. Capelletti*, L. Kovács, C. Mora*: FTIR spectroscopy of OH-induced defects in KTP single crystals. *Radiation Effects and Defects in Solids*, accepted for publication.

S.9. K. Lengyel, L. Kovács, G. Mandula, R. Rupp*: Kinetics of OH^- ions in nearly stoichiometric $LiNbO_3$ crystals. *Ferroelectrics*, accepted for publication.

S.10. S. Erdei*, R.G. Schlecht*, L. Kovács: Growth of PZN crystals with improved optical quality using the BSFT technique. *IEEE Transactions on Ultrasonics, Ferroelectrics, and Frequency Control*, accepted for publication.

S.11. G. Corradi, Th. Lingner*, A.B. Kutsenko*, V. Dierolf*, K. Polgár, J.-M. Spaeth* and W. von der Osten*: Magneto-optical studies of Er^{3+} in $LiNbO_3$. *Rad. Eff. Def. Solids*, accepted for publication.

S.12. L. Grigorjeva*, V. Pankratov*, D. Millers*, G. Corradi, K. Polgár: Relaxation of electronic excitations in LiNbO3 crystals. *Ferroelectrics*, accepted for publication

S.13. A. Watterich, L.A. Kappers*, O.R. Gilliam*, R.H. Bartram*, I. Földvári, L. Korecz: Paramagnetic and diamagnetic defects in e^- and UV-irradiated TeO_2. *Nucl. Instr. Meth. Phys. Res. B*, accepted for publication.

S.14. L. Malicskó, A. Watterich: Changes of OH^- bands induced by laser irradiation in $LiNbO_3$:Fe Single Crystals, *Nucl. Instr. Meth. Phys. Res. B*, accepted for publication.

S.15. D.Millers*, L.Grigorjeva*, V.Pankratov*, S.Chernov*, A.Watterich: Time-resolved spectroscopy of $ZnWO_4$. *Rad. Eff. Def. Solids*, accepted for publication.

S.16. R.T.Williams*, K.B.Ucer*, H.M.Yochum*, L.Grigorjeva*, D.Millers*, G.Corradi: Self-trapped electron and transient defect absorption in niobate and tungstate crystals. *Rad. Eff. Def. Solids*, accepted for publication.

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S.17. G. Mandula, K. Lengyel, L. Kovács, M. A. Ellabban*, R. A. Rupp*, M. Fally*: Thermal fixing of holographic gratings in nearly stoichiometric $LiNbO_3$ crystals. In: *International Conference on Solid State Crystals, Zakopane, Poland, Proceedings of SPIE*, **4412**, 226-230, 2001.

S.18. M. A. Ellabban*, G. Mandula, R. A: Rupp*, M. Fally*, E. Hartmann, L. Kovács, K. Polgár: Activation energy of thermal fixing in $LiNbO_3$: a comparative study. *Proceedings of SPIE*, accepted for publication.

See also R.11., T.17.

T. NONLINEAR AND QUANTUM OPTICS

P. Ádám, P. Domokos, A. Gábris[#], J. Janszky, A. Kárpáti[#], Zs. Kis, T. Kiss, Z. Kurucz[#], M. Koniorczyk[#], Sz. Szabó, V. Szalay

Quantum information, entanglement and teleportation. — We have introduced the one-complex-plane representation, a novel description of quantum states of two-mode light fields, which is a generalization of low-dimensional coherent state representations. We have shown, that this formulation is suitable for the treatment of entanglement and quantum teleportation of continuous variables. We have presented a unified description of both discrete and continuous variable quantum teleportation in terms of Wigner-functions. This is an application of phase space methods in quantum information theory, showing their adequacy even in the case of finite dimensional Hilbert-spaces. We have introduced an SU(3) theory of passive lossless optical six-ports, with special emphasis on few-photon interference applications such as optical state truncation and teleportation.

Cavity quantum electrodynamics and laser cooling. — We set up a systematic semiclassical model for the simulation of the dynamics of a single two-level atom strongly coupled to a driven high-finesse optical cavity. From the Fokker-Planck equation of the combined atom-field Wigner function we derived stochastic differential equations for the atomic motion and the cavity field. The corresponding noise sources were found to exhibit strong correlations between the atomic momentum fluctuations and the noise in the phase quadrature of the cavity field. The model provides an effective tool to investigate localisation effects as well as cooling and trapping times. In addition, we have studied the transition from a few photon quantum field to the classical limit of a large coherent field amplitude.

We calculated the loading efficiency and cooling rates in a bichromatic optical microtrap, where the optical potentials are generated by evanescent waves of cavity fields at a dielectric—vacuum interface. The cavity modified nonconservative dynamic light forces lead to efficient loading of the atoms as well as cooling without the need for spontaneous emission. Steady-state temperatures well below the trap depth, reaching the motional quantum regime, yield very long capturing times for a neutral atom.

Laser induced molecular dynamics. — We found that a beam of diatomic molecules scattered off a standing wave laser mode splits according to the rovibrational quantum state of the molecules. Our numerical calculation showed that single state resolution can be achieved by properly tuned, monochromatic light. The proposed scheme allows for selecting non-vibrating and non-rotating molecules from a thermal beam, implementing a laser Maxwell's demon to prepare a rovibrationally cold molecular ensemble.

Nuclear motion in molecules. — By making use of experimental vibrational spectroscopic data we have calculated the so called mode Grüneisen parameter of the OH stretching vibrational mode in 54 different hydrate, alkali halide, and oxide crystals. A new method of approximating the vibrational potential energy surfaces of molecules is the reconstruction method. We have shown how this method is related to the maximum entropy method. This relationship may allow us to describe quantitatively the importance the different sample points play in the reconstruction.

Nonlinear coherent states. — We have shown that the concept of nonlinear coherent states yields an efficient control of the vibrational state of a laser driven trapped ion. In particular

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we have pointed out that any state of an ion in a harmonic trap can be arbitrarily well approximated by a nonlinear coherent state that can be realized in many cases by applying a few laser fields.

Multilevel stimulated Raman adiabatic passage (STIRAP). — We have extended the STIRAP scheme in such a way that several ground states are coupled through an excited state by mutually coherent laser pulses. The ultimate aim of our study has been to find the pulse sequences that create prescribed coherent superposition states on the ground manifold. We have worked out two approaches:

(1) We have applied the optimal control theory (OCT) to this problem. We have found that OCT works surprisingly well: The numerical programs have provided not only the optimal pulse sequences but we have also managed to prove the robustness of the STIRAP scheme in our multistate case as well.

(2) We have worked out an analytic approach, too: The difficulty of the solution lays in the degeneracy of the Hamiltonian of the process. We have reduced the dimension of the system by separating the rapid and slow evolution in the process. In a restricted parameter space we have found an analytic solution that proved to be quite general.

Covariant coordinates in spacetime. — A great number of problems of relativistic position in quantum mechanics are due to the use of coordinates which are not inherent objects of spacetime, cause unnecessary complications and can lead to misconceptions. We apply a coordinate-free approach to rule out such problems. Thus it will be clear, for example, that the Lorentz covariance of position, required usually on the analogy of Lorentz covariance of spacetime coordinates, is not well posed and we show that in a right setting the Newton-Wigner position is Poincaré covariant.

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Grants and international cooperations

OTKA F 032341	Light-matter interaction in complex quantum systems (P. Domokos, 2000-2002)
OTKA T 034484	Application of nonclassical light in fundamental physical problems and in optical measurement methods (J. Janszky, 2001-2003)
OTKA F 032346	State reconstruction and preparation in quantum-optical systems (T. Kiss, 2000-2002)
OTKA T 034327	Reconstruction of vibrational potential energy surfaces of molecules, (V. Szalay, 2001-2003)

ICA1-CT-2000-70029 KFKI-CMRC Centre of Excellence, work package WP12: Growth and complex study of optical crystals (J. Janszky and I. Földvári)

TéT, Hungarian-Spanish Bilateral Intergovernmental S&T Cooperation E-10/2001: Calculation of the rotation-torsion spectrum of molecules with asymmetric top and asymmetric frame, and analysis of overlapping spectral bands by filter diagonalization (V. Szalay, 2001-2003)

HAS-SAS (Hungarian-Slovakian bilateral): Quantum optics (J. Janszky, 2000-2001)

Publications

Articles

T.1. P. Domokos, P. Horak*, and H. Ritsch*: Semiclassical theory of cavity-assisted atom cooling. *Journal of Physics B* **34**, 187-198 (2001).

T.2. P. Domokos and H. Ritsch*: Efficient loading and cooling in dynamic optical evanescent-wave microtraps. *Europhysics Letters* **54**, 306-312 (2001).

T.3. P. Domokos, T. Kiss, and J. Janszky: Selecting molecules in the vibrational and rotational ground state by deflection. *European Physical Journal D* **14**, 49-53 (2001).

T.4. P. Domokos, P. Horak* and H. Ritsch*: Semiclassical theory of cavity-assisted light forces on atoms and applications. *Progress of Physics* **49**, 935-940 (2001).

T.5. J. Janszky, A. Gábris, M. Koniorczyk, A. Vukics*, and P. Ádám: Coherent-state approach to entanglement and teleportation. *Progress of Physics* **49**, 993-1000 (2001).

T.6. J. Janszky, M. Koniorczyk, A. Gábris: One-complex-plane representation approach to quantum teleportation. *Physical Review A* **64**, 034302/1-4 (2001).

T.7. Z. Kis, W. Vogel*, L. Davidovich*, and N. Zagury*: SU(2) states of the motion of a trapped ion. *Physical Review A* **63**, 053410/1-7 (2001).

T.8. Z. Kis, W. Vogel*, and L. Davidovich*: Nonlinear coherent states of trapped-atom motion. *Physical Review A* **64**, 033401/1-10 (2001).

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T.12. S. Szabó, P. Ádám, A. Kárpáti, and J. Janszky: Phase optimized light in complex optical systems. *Progress of Physics* **49**, 1109-1116 (2001).

T.13. Z. Kis and S. Stenholm*: Nonadiabatic dynamics in the dark subspace of a multilevel stimulated Raman adiabatic passage process. *Physical Review A* **64**, 063406/1-10 (2001).

T.14. Z. Kis and S. Stenholm*: Measuring the density matrix by local addressing. *Physical Review A* **64**, 065401/1-4 (2001).

T.15. Z. Kis and S. Stenholm*: Optimal control approach for a degenerate STIRAP. *Journal of Modern Optics*, accepted for publication.

T.16. Sz. Farkas*, Z. Kurucz, and M. Weiner*: Poincare covariance of relativistic quantum position. *International Journal of Theoretical Physics*, accepted for publication

T.17. V. Szalay, L. Kovács, M. Wöhlecke*, E. Libowitzky*: Stretching potential and equilibrium length of the OH bond in solids. *Chemical Physics Letters*, accepted for publication.

Conference proceedings

T.18. M. Gangl*, P. Horak*, P. Domokos, and H. Ritsch*: Collective cooling of neutral particles in cavities without spontaneous emission. In: *Proceedings of MPLP 2000 (Symposium on Modern Problems of Laser Physics), Akademgorodok Novosibirsk, Russia*, Eds. S. I. Bagayev and V. I. Denisov, accepted for publication.

T.19. H. Ritsch*, P. Domokos, P. Horak*, M. Gangl*: Optical cooling in high-Q multimode cavities. In: *Proceedings of ICOL 2001*, accepted for publication.

T.20. J. Janszky, A. Gábris, M. Koniorczyk, A. Vukics*, J. Asboth*: One-complex-plane representation: a coherent state description of entanglement and teleportation. In: *Proceedings of the 7th International Conference on Squeezed States and Uncertainty Relations, NASA*, accepted for publication.

T.21. M. Koniorczyk and J. Janszky: Photon number conservation and photon interference. In: *Proceedings of the 1st International Workshop of RCO, Proc. of SPIE*, accepted for publication.

See also: P.7., P.10.

THE SZFKI AS THE HOST INSTITUTE OF THE CENTRE OF EXCELLENCE "KFKI-CMRC"

Our institute, together with the KFKI Atomic Energy Research Institute, the KFKI Research Institute for Particle and Nuclear Physics and the Research Institue for Technical Physics and Material Science established an organisation, the KFKI Condensed Matter Research Center (KFKI-CMRC) in order to coordinate the research activity in the field of condensed matter physics and applications at the KFKI campus. In 2000 the KFKI-CMRC became a **„Centre of Excellence"** within the 5th Framework programme of the European Union.

"Centres of Excellence" is part of a programme launched by the European Commission in order to contribute to the restructuring of the science and technology sector of the newly associated states. As many as 34 excellent research centers have been selected in these countries and will be supported to improve their links with other European centers through different types of activities, such as invitation of experienced scientists, training of Ph.D. students and post-doctoral researchers, organizing workshops and conferences, etc.

Our project started on the 1st of November 2000 and will commence on the 31st of October 2003. Twelve work packages and approximately 280 scientists belong to the Center. Our activities cover a broad spectrum of condensed matter research, that includes among others, the field of nuclear physics, theoretical and experimental solid state physics and optics, metal physics, liquid crystal research, materials science, advanced analytical methods etc. The projects coordinated by scientists of the Research Institute for Solid State Physics and Optics are the following:

— WP1 Enhancing regional users' access to the new Cold Neutron Facility at the Budapest Research Reactor (Dr. L. Rosta)

— WP7 Condensed matter theory (Pr. F. Iglói)

— WP8 Atomic level structural studies by photons and neutrons (Dr. Gy. Faigel)

— WP9 Nation-wide Co-operation for the Study of Non-equilibrium Metallic Materials (Dr. T. Kemény)

— WP11 Interaction of light with condensed matter (Dr. N. Éber)

— WP12 Growth and complex study of optical crystals (Pr. J. Janszky)

At the end of our first year as a Centre of Excellence we can conclude that the funding has helped in enhancing joint research with scientists from EU member and associated states.

In particular:

— We have employed 20 foreign scientists from 9 different countries as long term visitors for 60 months altogether;

— We have employed 32 foreign scientists who have visited our centre for a short period of time;

— 11 international conferences, workshops etc. were organised, six of which by the Research Institute for Solid State Physics and Optics;

— Durable equipments have been purchased for 23179 euro

These collaborations proved to be successful and we look forward for continuing these relationships with our guests in order to provide further advancement in their respective fields. We are trying to establish long lasting connections and aim for an international recognition of our achievemnets.

EDUCATION

Graduate and postgraduate courses, 2001

— Electrodynamics of continuous media (F. Woynarovich, ELTE[5])

— Completely integrable many body systems (F. Woynarovich, ELTE)

— Advanced Solid State Physics (J. Sólyom, ELTE)

— Statistical physics (F. Iglói, SZTE[6])

— Applications in statistical physics (F. Iglói, SZTE)

— Surface Magnetism (B. Újfalussy, ELTE)

— Magnetism I. (P. Fazekas, BMGE[7])

— Magnetism II. (P. Fazekas, BMGE)

— Advanced Solid State Physics (I. Tüttő, ELTE)

— Optical Properties of Solid State (I. Tüttő, ELTE)

— Metal Physics (J. Kollár, BMGE-ELTE)

— Solid state research I-II (I. Vincze, ELTE)

— Amorphous and crystalline materials (P. Deák*, S. Kugler* and T. Kemény, BMGE)

— Modern theory of nucleation (L. Gránásy, ELTE)

— Macromolecules (S. Pekker, ELTE)

— Spectroscopy and materials structure (K. Kamarás, BMGE)

— Methods in materials science (K. Kamarás, BMGE)

— Infrared and Raman spectroscopy (K. Kamarás, BMGE)

— Physics of liquid crystals and polymers (Á. Buka and N. Éber, ELTE)

— Pattern formation in complex systems (Á. Buka, ELTE)

— Crystalline and amorphous materials (Á. Buka, BMGE)

— Liquid crystals as matrix materials for display devices (K. Fodor-Csorba, ELTE)

— Nanophase metals: Magnetism and electrical transport (I. Bakonyi, ELTE)

— Advanced material technology (G. Konczos, BMGE and ELTE)

— NMR spectroscopy (K. Tompa, BMGE)

— Group theory in solid state research (G. Kriza, BMGE)

— Superconductivity (G. Kriza, BMGE)

— Neutron scattering in condensed matter (L. Cser, ELTE)

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[5] ELTE = Loránd Eötvös University, Budapest

[6] SZTE = University of Szeged

[7] BMGE = Budapest University of Technology and Economics

— Disorder in condensed phases (L. Pusztai, ELTE)

— Neutrons in condensed matter research (L. Pusztai, BMGE)

— Introduction to ultrafast optics (R. Szipőcs, ELTE)

— Optical methods in solid state physics (Z. Szentirmay, ELTE).

— Physics of Amorphous Matter I. (M. Koós and I. Pócsik, SZTE)

— Physics of Amorphous Matter II. (I. Pócsik and M. Koós, SZTE)

— Crystal Physics of Optical Crystals (I. Földvári, Á. Péter, BMGE)

— Crystal growth from the melts and various special techniques (in: Crystalline and Amorphous Materials, K. Polgár, BMGE)

— Growth, orientation and processing of nonlinear optical crystals (in: Applied Lasertechnics, K. Polgár, Á. Péter, I. Földvári, BMGE)

— Theories of Crystal Growth (L. Malicskó, BMGE)

— Microscopy in Materials Science (L. Malicskó, BMGE)

— Technical application of crystals (E. Hartmann, BMGE)

— The characterization of crystals (E. Hartmann, BMGE)

— The generalization of crystallographic groups (E. Hartmann, ELTE)

— Statistical quantum optics (J. Janszky ELTE)

— Thermodynamics and statistical physics (P.Ádám, PTE[8])

— Electrodynamics (P. Ádám, PTE)

— Mechanics (P. Ádám, PTE)

— Quantum mechanics (P. Ádám, PTE)

— Radiation theory (P. Ádám, PTE)

— Vector calculus II (A. Kárpáti, PTE)

Laboratory practice and seminars

— Solid State Physics seminar (J. Sólyom, ELTE)

— Laboratory for solid state physics, Preparation and crystallization of metallic glasses (I. Vincze, ELTE)

— Infrared and Raman spectroscopy laboratory practice, (K. Kamarás, BMGE)

— Basic experimental physics (L. Gránásy, BMGE)

— Atomic and molecular physics laboratory, (K. Kamarás, ELTE)

— Experiments on liquid crystals (Á. Buka, ELTE)

— NMR spectroscopy (K. Tompa, ELTE and BMGE)

[8] PTE = University of Pécs

— Physical Chemistry Laboratory Practice (L. Péter, ELTE)

— Advanced solid state physics laboratory (I. Pethes and L. Németh, ELTE and BMGE)

— Neutron scattering (L. Rosta, BMGE)

— Neutron scattering and hands-on-training at BRR (L. Cser, Gy. Török, E. Rétfalvi, BMGE)

— Neutron scattering in materials research (L. Rosta, ME[9])

— Neutron detectors (E. Rétfalvi, BMGE)

— International graduate training in neutron scattering (L. Cser, Gy. Török, M. Avdeev, Hungarian-Austrian Fund)

— Computing in chemistry (L. Pusztai, ELTE)

— Medical application of lasers (Z. Gy. Horváth, Medical Laser Center)

— Electrodynamics (K. Lengyel, PTE)

— Thermodynamics and statistical physics (K. Lengyel, PTE)

— Elementary calculus and linear algebra (K. Lengyel, PTE)

— Elementary calculus and linear algebra (M. Koniorczyk, PTE)

— Vector calculus (A. Kárpáti, PTE)

Diploma works

— Sz. Németh (BMGE): Electrohydrodynamic convective patterns in nematic liquid crystals. (Consultants: Á. Buka, N. Éber)

— Ákos Bányász (ELTE): Computer controlled pump-probe experimental setup for time resolved spectroscopy using a tunable, fs pulse Ti:sapphire laser (Consultant: R. Szipőcs)

— Gábor Dancs (ELTE): Evaluation of experimental data obtained by time resolved femtosecond spectroscopy (Consultant: R. Szipőcs)

— Miklós Füle (SZTE): Optical Absorption Investigation of Hydrogenated Amorphous Carbon Films (Consultant: M. Koós)

— A. Gábris (ELTE): EPR pairs coherent-state basis (Consultant: J. Janszky)

— Z. Kurucz (ELTE): Quantum state transformation via teleportation (Consultant: J. Janszky)

Ph. D. students

Z. Jurek (BMGE): Atom resolution imaging of non-periodic systems (Supervisor: Gy. Faigel)

Sz. Németh (BMGE): Instabilities and convective patterns in liquid crystals. (Supervisor: Á. Buka)

[9] ME = University of Miskolc

H. Nádasi (ELTE): Banana shaped liquid crystals and their physico-chemical properties. (Supervisor: K. Fodor-Csorba)

É. Fazakas (ELTE): Preparation of bulk amorphous alloys by mechanical alloying (Supervisor: L.K. Varga)

L. Németh (BMGE): NMR study of low-dimensional metals (Supervisor: G. Kriza)

A. Kákay (ELTE): Magnetic nanocomposites: modelling and experiments (Supervisor: L.K. Varga)

P. Matus (BMGE): NMR study of metals with correlated electronic system (Supervisor: G. Kriza)

I. Pethes (BMGE): Experiments on moving glasses (Supervisor: G. Kriza)

I. Varga (BMGE): Magnetic domain contrast studies and image processing by SEM (Supervisor: L. Pogány)

L. Almásy: Investigation of liquid mixtures by neutron scattering (Supervisor: L. Cser)

M. Avdeev: SANS Study of Soft Condensed Matter (Supervisor: L. Rosta)

A. Len: Small angle neutron scattering study of sintered materials (Supervisor: L. Rosta)

E. Rétfalvi: Irradiation damage study of materials of technological importance by neutron scattering technique (Supervisor: L. Rosta)

G. Vaspál: Applied Neutron Optics (Supervisor: L. Cser)

Z. Somogyvári (BMGE): Magnetic and atomic structure investigations by neutron diffraction (Supervisor: E. Sváb)

K. Mocsár (BMGEG): Producing high-intensity ultrashort laser pulses with a solid state laser system for experimental investigation of light-matter interaction. (Supervisor : Gy. Farkas)

P. Hartmann (ELTE): Elementary processes in gas discharges (Supervisor: Z. Donkó)

P. Horváth (ELTE): Metal-ion lasers (Supervisor: K. Rózsa)

K. Kutasi (PTE): Modelling of glow discharges (Supervisor: Z. Donkó)

G. Bánó (SZTE): Cathode sputtered and heated Zn lasers in high voltage hollow cathode discharges (Supervisor: K. Rózsa)

S. Lakó (SZTE): Nonlinear frequency conversion of femtosecond laser pulses (Supervisor: R. Szipőcs)

K. Szőcs (SE): Photosensitisation of *Escherichia coli B.* bacteria by endogenous porphyrin derivatives (Supervisor: R. Szipőcs)

M. Füle (SZTE): Optical Properties of Graphitic Carbon Nano-Structures (Supervisor: M. Koós)

Z. Lipp (BMGE): Laser Doppler velocimetry (Supervisor: P. Jani)

A. Nagy (ELTE): Investigation of the optical properies of airborne particles (Supervisor A. Czitrovszky)

M. Veres (SZTE): Physical Properties of Graphitic Carbon Nano-Structures (supervisor I. Pócsik)

H. Moussambi (Université de Metz): (Hungarian co-leader: K. Polgár)

K. Lengyel (PTE): Study of OH^- ion absorption in non-linear optical crystals (Supervisor: L. Kovács)

A. Gábris (SZTE): Nonlinear photonic crystals and quantum optical processes therein (Supervisor: J. Janszky)

A. Kárpáti (PTE): Quantum phenomena in photonic band-gap structures (Supervisor: P. Ádám)

M. Koniorczyk (PTE): Nonlocality in quantum optical systems (Supervisor: J. Janszky)

Z. Kurucz (SZTE): Quantum state manipulations and quantum information theory (Supervisor: J. Janszky)

Dissertations

T. Kemény: Atomic volume dependence of the magnetic properties of iron alloys (D.Sc., HAS)

A Jákli: Ferroelectricity in liquid crystals (D.Sc., HAS)

V. Szalay: New methods to solving the vibrational Schrödinger equation of molecules: Discrete variable representations and distributed approximating functions (D.Sc., HAS)

S. Varró: Photon-electron interactions in intense laser fields, (University of Szeged) Habilitationsschrift,

E. Mátyus-Szabó: Mesomorphism of new type banana shaped liquid crystals. (Ph.D. ELTE)

B. Varga: Change of soft magnetic properties in Fe-B-Si based aloys during amorphous-to-nanocrystalline transformation (Ph.D., BMGE)

R. Szipőcs: Dispersive properties of dielectric high reflectors and their use in femtosecond pulse lasers (Ph.D., SZTE, Szeged)

Zs. Szaller: Reactions and phases in the TeO_2 rich part of the system of Bi_2O_3-TeO_2. (Ph.D. ELTE)

Awards

— J. Janszky, Elected as Corresponding Member of the Hungarian Academy of Sciences

— Gy. Faigel, Elected as Corresponding Member of the Hungarian Academy of Sciences

— G. Fáth, Bolyai Grant (1999-2002)

— Ö. Legeza, Bolyai Grant (2000-2003)

— K. Penc, Bolyai Grant (1999-2002)

— K. Penc, OTKA post-doctoral grant D 32689

— J. Sólyom, Széchenyi Professorship (1999-2002)

— J. Kollár, Award of the Hungarian Academy of Sciences (2001)

— J. Kollár, Széchenyi Professorship (2000-2003)

— F. Woynarovich, Széchenyi Professorship (2000-2003)

— L. Gránásy, Széchenyi Professorship (1999-2003)

— M. Tegze, Publication Award of RISSPO (2001)

— K. Kamarás, Széchenyi Professorship (1998-2002)

— G. Oszlányi, Bolyai Grant (1998-2001)

— Á. Buka, Széchenyi Professorship (1998-2001)

— G. Kriza, Széchenyi Professorship (1999-2002)

— M. Bokor, Bolyai Grant (2001-2004)

— L. Pusztai, Széchenyi Professorship (2000-2003)

— Z. Donkó, Bolyai Grant (1998-2001)

— R. Szipőcs, Bolyai Grant (1999-2002)

— A. Czitrovszky, Price for Invention, of the Hungarian Academy of Sciences (2001)

— I. Földvári: Széchenyi Professorship, (2000-2003)

— L. Bencs: Postdoctroral grant, Belgian Office for Scientific, Technical and Cultural Affairs (2001-2002)

— J. Janszky, Széchenyi Professorship (1998-2001)

— Z. Kis, Bolyai Grant (2001-2003)

CONFERENCES

— **Annual Meeting of the Research Training Network "Computational Magnetoelectronics", 27-30, September 2001, Budapest, Hungary**. The first Annual Meeting of this Network was organized by the Theoretical Solid State Physics Department of the Research Institute for Solid State Physics and Optics. Over eighty members of the eight national nodes came together to review their common activity within the Network during the first year and to discuss further progress. In addition,

several leading researchers of the field were invited. In total fifty-five oral contributions, among them six review talks, were reported.

— **Application of Atomic Resolution Methods for the Study of Advanced Materials**, International Summer School and Workshop, August 28-September 1, 2001, Budapest, Organised jointly by the Loránd Eötvös University and the Budapest Condensed Matter Research Centre – Centre of Excellence WP9. 40 participants (including 20 Ph.D. students) attended the school. The lectures of prominent international experts from Germany, France, England and Japan were aimed to give a broad overview of research tools applied in the study of different advanced materials (e.g. nanostructures).The topics included: element specific studies of magnetization by x-ray, high resolution neutron and electron microscopy techniqes, micro-thermal analysis, atomic resolution analytical methods and positron annihilation spectroscopy. As to the contribution of our institute, G. Faigel delivered the lecture: Atomic Resolution X-ray Methods The lively discussions after the lectures and also at the social programs hint to further intensive co-operations among the participants

— International workshop on **Vortex Dynamics and Dissipation in High T_c Superconductors** (Budapest, Hungary, April 26-29, 2001). Organizers: B. Sas and G. Kriza (Centre of Excellence, WP9). Number of participants: 35. The aim of the workshop was to bring together scientists working in the field of vortex dynamics and possible sources of dissipation in the mixed state of high-T_c superconductors. About 6 lectures a day and lots of free discussion were held. The topics discussed include: Transport measurements (critical current, dissipation beyond the critical current, Hall effect); magnetization measurements; intrinsic Josephson junctions; metastability, aging.

— Workshop on **Electrodeposited Nanostructures** (Budapest, Hungary, May 25, 2001). Organizers: I. Bakonyi and L. Péter. The lectures were given by the organizers and by the 3 invited British scientists from the University of Bristol and the University of Newcastle. The lectures dealt with the pulse-plated nanostructures, with special reference to the electrochemical issues of the preparation magnetic/non-magentic multilayers with GMR behaviour. About 20 scientists from the Research Institute for Solid State Physics and Optics as well as from other research institutes of the Hungarian Academy of Sciences participated in the workshop which was closed with an informal round-table discussion about current issues of the field and about prospective collaboration areas of the workshop participants.

— A workshop entitled "**New Opportunities in Single Crystal Spectroscopy with Neutrons** " was organised between April 19-22, 2001, at Lake Balaton (Révfülöp), Hungary, in order to conclude the main achievements in the field and to provide a forum for the dissemination of results and for training of young researchers. The workshop had also some tutorial character with the aim to enhance this kind of activity for newcomers in this field.

— **Fourth Annual Meeting of the COST Action P2 "Applications of nonlinear optical Phenomena" and Workshop on $LiNbO_3$**, Budapest, 16-19 May, 2001 (I. Földvári, chair, L. Kovács, secretary). The COST Action P2 was established to support research in an actively developing area of applied optics, the field related to nonlinear phenomena in optical materials. The program has covered all aspects of the 7 active working projects. A specific section was devoted to the most widely used nonlinear optical material, $LiNbO_3$. Beside the 12 invited lectures, 72 contributing presentations

have been submitted. The number of the registered participants was 106, from 22 countries. The research program was divided to 12 oral and 2 poster sessions:

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